

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
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
3290	GROMACS	Task	Resolved	Normal	Require CMake >= 3.12		04/14/2020 02:45 PM	2021-refactoring
3295	GROMACS	Feature	New	Normal	Expand gmxapi.modify_input use cases.	Eric Irrgang	01/16/2020 05:13 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
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
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
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

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3374	GROMACS	Feature	New	Normal	SimulationInput abstraction		03/03/2020 05:32 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
3416	GROMACS	Task	New	Normal	Port post-submit matrix to Gitlab CI	Joe Jordan	03/16/2020 05:50 PM	2021-refactoring
3266	GROMACS	Bug	New	High	gmx density show wrong symmetrize density profile using -symm?	Super duper	02/28/2020 08:24 AM	2020.2
2667	GROMACS	Feature	New	Normal	Suggested steps for calculating entropy in solution and binding	David van der Spoel	03/01/2020 01:35 PM	2020.2
2723	GROMACS	Task	New	Normal	Update mdrun-performance.rst to clearly express the nature of task	Joe Jordan	02/27/2020 11:07 AM	2020.2
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
3071	GROMACS	Bug	Accepted	Normal	complex.nbnxn-ljpmc-LB-geometric failing with OpenCL timing debug mode assertions	Szilárd Páll	02/25/2020 03:39 PM	2020.2
3125	GROMACS	Bug	Resolved	Normal	OpenCL on Volta and Turing broken		02/27/2020 11:01 AM	2020.2
3294	GROMACS	Bug	New	Normal	multiple tests fail on fedora 31	Paul Bauer	02/28/2020 03:12 PM	2020.2
3304	GROMACS	Bug	New	Normal	Failure in Log Output for Expanded Ensemble Weights using Simulated Tempering in GROMACS 2019.5	Michael Shirts	03/01/2020 03:23 PM	2020.2
3334	GROMACS	Bug	New	Normal	Check for DD when increasing rlist is broken	Berk Hess	02/25/2020 03:28 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
3408	GROMACS	Bug	Fix uploaded	Normal	Gmxapi* tests segfault in rpmbuild	Eric Irrgang	03/23/2020 01:27 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
3050	GROMACS	Bug	New	Low	Fix tests on Solaris	Vedran Miletic	02/27/2020 11:05 AM	2020.2
3380	GROMACS	Bug	Resolved	Low	IBM VSX checks fail with gcc-10	Erik Lindahl	04/30/2020 01:30 PM	2020.2
3093	GROMACS	Task	In Progress	High	rework GPU direct halo-exchange related force reduction complexities		02/14/2020 11:35 AM	2021-infrastructure-stable
3160	GROMACS	Feature	Fix uploaded	High	implement direct comm for different src/target memory spaces	Alan Gray	02/14/2020 11:28 AM	2021-infrastructure-stable
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
2395	GROMACS	Task	In Progress	Normal	break up commrec	Mark Abraham	12/15/2019 11:51 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
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
2706	GROMACS	Task	Accepted	Normal	Rework classic QM/MM interface		12/02/2019 01:45 PM	2021-infrastructure-stable

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2795	GROMACS	Task	New	Normal	Incorporate regressiontests into core gromacs		12/02/2019 01:44 PM	2021-infrastructure-stable
2833	GROMACS	Task	New	Normal	Update topology datastructures	Paul Bauer	12/02/2019 01:43 PM	2021-infrastructure-stable
2875	GROMACS	Task	Accepted	Normal	SIMD version of the free-energy kernel	Berk Hess	12/02/2019 01:44 PM	2021-infrastructure-stable
2916	GROMACS	Task	New	Normal	Decide future of symtab	Paul Bauer	09/06/2019 02:35 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
2994	GROMACS	Feature	New	Normal	Data flow topology in gmxapi 2020		12/11/2019 11:33 AM	2021-infrastructure-stable
2996	GROMACS	Feature	In Progress	Normal	gmxapi execution model	Eric Irrgang	12/10/2019 01:57 PM	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
3035	GROMACS	Task	New	Normal	Provide central logger in wrapper binary	Paul Bauer	09/06/2019 02:34 PM	2021-infrastructure-stable
3038	GROMACS	Feature	New	Normal	Improvements to MD plugin development environment	Eric Irrgang	12/10/2019 01:58 PM	2021-infrastructure-stable
3072	GROMACS	Task	New	Normal	Use gmx::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
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
3117	GROMACS	Feature	New	Normal	Coulomb FEP PME on GPU	Magnus Lundborg	02/17/2020 03:58 PM	2021-infrastructure-stable
3130	GROMACS	Task	New	Normal	Interim handling of gmxapi data references.	Eric Irrgang	12/11/2019 11:26 AM	2021-infrastructure-stable
3131	GROMACS	Task	New	Normal	support ccache with clang-tidy	Mark Abraham	12/20/2019 08:20 AM	2021-infrastructure-stable
3133	GROMACS	Task	In Progress	Normal	Cookiecutter for sample_restraint	Eric Irrgang	12/10/2019 01:59 PM	2021-infrastructure-stable
3136	GROMACS	Bug	New	Normal	gmxapi.operation data flow topology unclear or incomplete	Eric Irrgang	12/11/2019 11:25 AM	2021-infrastructure-stable
3140	GROMACS	Feature	New	Normal	Allow explicit input definition for gmxapi.operation function wrapper	Eric Irrgang	12/10/2019 02:00 PM	2021-infrastructure-stable
3141	GROMACS	Bug	New	Normal	gmxapi File placeholders missing from beta release	Eric Irrgang	12/10/2019 02:02 PM	2021-infrastructure-stable
3147	GROMACS	Feature	New	Normal	gmxapi workflow checkpointing	Eric Irrgang	10/15/2019 06:18 PM	2021-infrastructure-stable
3148	GROMACS	Feature	New	Normal	Roadmap for gmxapi filesystem interactions.	Eric Irrgang	10/15/2019 06:23 PM	2021-infrastructure-stable
3150	GROMACS	Bug	New	Normal	gmxapi data type annotations are confusing and inadequate	Eric Irrgang	10/22/2019 03:08 PM	2021-infrastructure-stable
3152	GROMACS	Feature	New	Normal	Infrastructure and patterns for expressing public interfaces		01/09/2020 05:19 PM	2021-infrastructure-stable

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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
3171	GROMACS	Task	New	Normal	schedule CPU H2D force contribution in separate stream		12/20/2019 08:33 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
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
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
3220	GROMACS	Task	New	Normal	change rolling pruning scheduling with GPU update		02/25/2020 03:41 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
3229	GROMACS	Task	New	Normal	Move checkpointing to the beginning of the MD step		01/16/2020 04:31 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
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
3264	GROMACS	Task	New	Normal	Break up MdrunMpiTests	Paul Bauer	12/23/2019 11:44 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
3272	GROMACS	Task	New	Normal	Port complete CI testing to Gitlab	Paul Bauer	02/27/2020 11:04 AM	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
3275	GROMACS	Task	New	Normal	Document Gitlab CI instead of Jenkins and releng	Paul Bauer	03/09/2020 05:55 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
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
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
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

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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
3363	GROMACS	Feature	New	Normal	Improve FEP testing	Pascal Merz	03/01/2020 03:22 PM	2021-infrastructure-stable
3379	GROMACS	Feature	New	Normal	C++ API for simulation input and output		02/28/2020 10:38 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
3394	GROMACS	Feature	New	Normal	improve gmxapi error handling	Eric Irrgang	02/24/2020 11:45 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
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
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

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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
2481	GROMACS	Task	New	Low	Update gmx report-methods to write more method information		12/02/2019 01:22 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
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
3260	GROMACS	Task	New	Low	keep up to with mdspan reference implementation	Christian Blau	12/20/2019 01:16 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
2453	GROMACS	Task	Resolved	High	PME OpenCL porting effort	Aleksei Lupinov	12/20/2019 12:18 PM	2021
3082	GROMACS	Task	New	High	move launch/synchronization points to clarify task dependencies		12/27/2019 04:21 PM	2021
868	GROMACS	Feature	In Progress	Normal	Implement parallelization support to analysis framework	Kevin Boyd	12/20/2019 11:59 AM	2021
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
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
2169	GROMACS	Task	New	Normal	remove 'continuation' mdp option		12/29/2019 10:31 AM	2021
2224	GROMACS	Feature	New	Normal	Proposed feature: conditional stop	Vedran Miletic	12/20/2019 12:11 PM	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
2425	GROMACS	Task	New	Normal	testing multisim with multiple ranks per simulation	Mark Abraham	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
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
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
2710	GROMACS	Feature	New	Normal	Separate dwdl for each molecule (of couple-moltype) when running FEP		12/27/2019 04:41 PM	2021
2766	GROMACS	Task	In Progress	Normal	Improve hardware option selection	Kevin Boyd	12/20/2019 02:34 PM	2021

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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
2774	GROMACS	Feature	New	Normal	Refactor shell code into its own integrator	David van der Spoel	12/27/2019 04:05 PM	2021
2806	GROMACS	Feature	New	Normal	SIMD algorithms for ARM SVE // nobnonded cluster and others		12/27/2019 03:59 PM	2021
2834	GROMACS	Task	In Progress	Normal	C++ matrix classes	Christian Blau	12/29/2019 10:32 AM	2021
2839	GROMACS	Task	New	Normal	make module and file naming consistent		01/16/2020 05:11 PM	2021
2877	GROMACS	Task	New	Normal	use gmx::Options more	Mark Abraham	12/20/2019 01:22 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
2944	GROMACS	Feature	New	Normal	Roadmap for thermostats / barostats in new propagation/integration scheme	Michael Shirts	12/27/2019 04:00 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
3057	GROMACS	Task	New	Normal	re-enable fusion on Power8/9	Szilárd Páll	12/27/2019 04:22 PM	2021
3062	GROMACS	Task	New	Normal	add twin cut-off mdrun test		12/27/2019 04:22 PM	2021
3064	GROMACS	Task	New	Normal	add test for perturbed bonded forces		12/27/2019 04:22 PM	2021
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
3114	GROMACS	Feature	New	Normal	Improve GPU update-constraints module	Artem Zhmurov	02/10/2020 04:30 PM	2021
3119	GROMACS	Task	New	Normal	clang-tidy coverage of parallelizaton 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
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
3224	GROMACS	Task	New	Normal	add regression test case large enough to miscalculated GPU grid launch cases		12/20/2019 01:18 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

#	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
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
3356	GROMACS	Task	New	Normal	Expose setting of random seed to API		01/29/2020 06:16 PM	2021
3371	GROMACS	Feature	New	Normal	Control FEP using AWH	Magnus Lundborg	02/06/2020 02:20 PM	2021
3410	GROMACS	Feature	New	Normal	Random Acceleration Molecular Dynamics (RAMD)	Bernd Doser	03/05/2020 03:22 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
1985	GROMACS	Bug	Fix uploaded	Low	CUDA build system refactoring awaiting review		12/20/2019 12:07 PM	2021
2192	GROMACS	Bug	Accepted	Low	grompp should read floats (e.g charge) from data files to double, to avoid accumulating round-off error	Berk Hess	12/20/2019 12:11 PM	2021
2695	GROMACS	Task	New	Low	bonded GPU module timing		12/27/2019 04:40 PM	2021
2832	GROMACS	Bug	New	Low	PaddedVector move operations broken	Mark Abraham	12/28/2019 10:40 AM	2021
2071	GROMACS	Task	In Progress	High	Low accuracy default settings yield incorrect liquid densities	Berk Hess	01/05/2018 03:32 PM	
2519	GROMACS	Task	New	High	Improve/remove PME OpenCL kernel barriers		02/15/2019 06:34 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	
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	
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	
2637	GROMACS	Bug	New	High	gmx solvate tears apart molecules		09/11/2018 07:43 PM	
2792	GROMACS	Task	New	High	Improvement of PME gather and spread CUDA kernels		03/18/2020 03:57 PM	
2915	GROMACS	Feature	In Progress	High	GPU direct communications		02/14/2020 12:48 PM	
3210	GROMACS	Bug	New	High	rerun does not reproduce dVcoul/dl		12/27/2019 10:45 AM	
3262	GROMACS	Task	New	High	Trjconv - dimer protein-ligand		12/20/2019 09:26 PM	
3370	GROMACS	Task	New	High	Further improvements to GPU Buffer Ops and Comms		03/04/2020 01:38 PM	
2099	Support Platforms	Feature	New	High	sharing accounts/credentials		12/06/2017 08:11 PM	
2188	TNG trajectory library	Feature	Resolved	High	Masses missing from TNG specification	Magnus Lundborg	06/13/2017 05:08 PM	
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	

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
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	
867	GROMACS	Task	In Progress	Normal	Update Doxygen documentation for C++ code	Teemu Murtola	07/11/2016 08:28 PM	
869	GROMACS	Task	In Progress	Normal	Make analysis data histogramming and multipoint data easier to use in parallel	Teemu Murtola	07/11/2016 08:28 PM	
920	GROMACS	Task	In Progress	Normal	Add test framework for trajectory analysis modules	Teemu Murtola	07/11/2016 08:27 PM	
921	GROMACS	Feature	Blocked, need info	Normal	Default index groups and selections		07/11/2016 08:27 PM	
948	GROMACS	Task	New	Normal	C++ thread synchronization primitives	Sander Pronk	07/11/2016 08:24 PM	
950	GROMACS	Feature	New	Normal	Path/directory/filename handling in Gromacs		07/11/2016 08:24 PM	
1010	GROMACS	Task	In Progress	Normal	Better support for multiple AnalysisData datasets	Teemu Murtola	07/11/2016 08:23 PM	
1017	GROMACS	Task	New	Normal	C++ Vector/Matrix classes		07/11/2016 08:23 PM	
1028	GROMACS	Feature	New	Normal	Tool to calculate fraction of native contacts during simulation		11/01/2012 10:27 PM	
1056	GROMACS	Task	Accepted	Normal	status of fft5d_threads and fftw3_threads functionality	Mark Abraham	07/11/2016 08:21 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	
1190	GROMACS	Bug	New	Normal	Use of FORCE in setting cached variables	Mark Abraham	06/17/2014 06:09 AM	
1192	GROMACS	Feature	Accepted	Normal	Add support for Verlet scheme with Buckingham	Berk Hess	07/11/2016 08:19 PM	
1214	GROMACS	Task	New	Normal	Keep track of important changes for Changelog	Mark Abraham	06/26/2013 11:24 AM	
1246	GROMACS	Task	New	Normal	expanded ensemble .tpr cannot be rerun	Michael Shirts	06/19/2015 01:56 PM	
1303	GROMACS	Feature	New	Normal	Adding lambda dependent distance for pull code	Michael Shirts	07/11/2016 08:18 PM	
1323	GROMACS	Task	New	Normal	determine future of existing tools for	David van der Spoel	12/04/2018 11:53 AM	
1328	GROMACS	Feature	Accepted	Normal	Names for selection positions		07/11/2016 08:15 PM	
1332	GROMACS	Feature	In Progress	Normal	Supporting multiple end states instead of just A and B	Michael Shirts	06/05/2018 03:58 PM	
1354	GROMACS	Bug	New	Normal	Constant acceleration NEMD is broken.	David van der Spoel	01/09/2019 04:42 PM	
1422	GROMACS	Feature	New	Normal	CSH angle incorrect with GROMOS force field and virtual sites	David van der Spoel	06/12/2014 12:01 AM	
1442	GROMACS	Bug	Feedback wanted	Normal	Not consistent solvation free energies differences	Michael Shirts	07/11/2016 08:13 PM	

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
1448	GROMACS	Bug	New	Normal	multiple successive crashes during REMD can lead to .log files that do not represent the actual replica exchanges to match the .xtc files (complicating demultiplexing)	Mark Abraham	06/23/2016 03:15 PM	
1489	GROMACS	Feature	New	Normal	Don't solely rely on filename extension		04/30/2014 05:23 AM	
1490	GROMACS	Task	New	Normal	Usage of forward declarations vs typedef vs #include	Mark Abraham	01/21/2015 10:23 AM	
1500	GROMACS	Feature	New	Normal	Post-5.0 feature clean-up plan	Mark Abraham	08/26/2019 03:47 PM	
1505	GROMACS	Task	New	Normal	improve handling of logging	Mark Abraham	01/02/2019 06:06 PM	
1511	GROMACS	Feature	Accepted	Normal	add PDBx (ie mmCIF) support		10/05/2018 07:14 PM	
1515	GROMACS	Task	New	Normal	improve g_bar output	Szilárd Páll	07/11/2016 08:10 PM	
1523	GROMACS	Task	New	Normal	add missing code-paths to CUDA emulation kernel		07/11/2016 08:09 PM	
1562	GROMACS	Feature	New	Normal	introducing a Monte Carlo framework (first application: MC barostat)	Michael Shirts	07/11/2016 08:08 PM	
1583	GROMACS	Bug	New	Normal	gmx msd with mol flag requires excessive memory		12/18/2017 03:34 PM	
1618	GROMACS	Bug	In Progress	Normal	g_protonate segfaults unconditionally	Erik Lindahl	08/17/2015 02:10 PM	
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	
1648	GROMACS	Bug	Feedback wanted	Normal	Atoms with zero LJ parameters but partial charges appear to cause crashes in free energy calculations when perturbed in the presence of other charges	Michael Shirts	06/25/2015 06:07 AM	
1652	GROMACS	Feature	New	Normal	Decide how to represent multiple lambda states internally	Michael Shirts	06/05/2018 03:58 PM	
1653	GROMACS	Feature	New	Normal	Decide how to represent multiple lambda states in the .top file and how to parse them	Michael Shirts	06/05/2018 03:58 PM	
1654	GROMACS	Feature	New	Normal	How to carry out movement between chemical end states in a multiple end state framework?	Michael Shirts	07/11/2016 08:05 PM	
1655	GROMACS	Bug	New	Normal	g_membed and box type		12/09/2014 01:33 PM	
1658	GROMACS	Feature	New	Normal	Electrostatics treatment for multiple lambda sites	Berk Hess	07/11/2016 08:05 PM	
1667	GROMACS	Bug	New	Normal	gmx convert-tpr writes wrong number of mol in output tpr	David van der Spoel	06/27/2016 08:29 PM	
1670	GROMACS	Feature	New	Normal	create mdrun option checking mini-tool		06/23/2016 04:06 PM	
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	
1786	GROMACS	Task	New	Normal	Python style standards in developer docs	Peter Kasson	12/26/2019 03:15 PM	
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	

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
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	
1843	GROMACS	Bug	In Progress	Normal	pbcs=xy with 2 walls floating point exception with the verlet scheme	Berk Hess	10/31/2016 11:35 AM	
1849	GROMACS	Feature	New	Normal	expanded ensemble -- Adaptive Integration Method	Christopher Mirabzadeh	07/11/2016 08:01 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	
1864	GROMACS	Feature	New	Normal	write tng files with energies	Magnus Lundborg	07/11/2016 08:00 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	
1934	GROMACS	Bug	New	Normal	QMMM with ORCA: memory leaks, buffer overflows and much more		07/10/2016 09:26 AM	
1947	GROMACS	Task	New	Normal	Consider fixing corner case in TinyXML2	Mark Abraham	04/19/2016 01:40 AM	
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	
2020	GROMACS	Bug	New	Normal	Possible issue with md-vv integrator	Mark Abraham	03/11/2017 08:30 AM	
2039	GROMACS	Bug	New	Normal	mdrun -pinstride defaults are too confusing		12/13/2017 04:14 AM	
2045	GROMACS	Task	New	Normal	API design and language bindings	Peter Kasson	01/29/2020 03:59 PM	
2048	GROMACS	Task	New	Normal	C++11: CUDA dependency on general headers		09/07/2016 10:30 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	
2080	GROMACS	Feature	New	Normal	add grompp warning for suitability for domain decomposition		11/23/2016 03:03 PM	
2089	GROMACS	Task	New	Normal	Encourage code review		01/10/2017 12:03 AM	

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
2090	GROMACS	Feature	New	Normal	redirecting stdout or stderr for testing	Mark Abraham	12/15/2016 03:15 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	
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	
2126	GROMACS	Feature	New	Normal	implement native CUDA support in CMake		10/29/2019 09:03 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	
2185	GROMACS	Task	New	Normal	add docs on MPI + CUDA w/wo MPS		05/24/2017 05:17 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	
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	
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-tpr 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	
2238	GROMACS	Task	In Progress	Normal	GPU emulation mode support for rolling pruning missing	Berk Hess	12/21/2017 03:21 PM	
2239	GROMACS	Feature	New	Normal	split libgromacs into base and full		01/07/2019 01:47 AM	
2248	GROMACS	Feature	New	Normal	Label all SIMD functions as pure/nodiscard		02/04/2019 04:49 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	
2283	GROMACS	Feature	New	Normal	Force distribution analysis	Bernd Doser	10/27/2017 11:44 AM	
2289	GROMACS	Feature	New	Normal	gmx spatial add ability to perform over multiple reference structures		11/08/2017 12:31 AM	

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
2294	GROMACS	Task	New	Normal	Require identical hardware on nodes on parallel runs		11/19/2017 08:54 PM	
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	
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	
2451	GROMACS	Feature	Resolved	Normal	Linear virtual sites with fixed distance	David van der Spoel	09/16/2019 01:15 PM	
2452	GROMACS	Task	In Progress	Normal	Reduce data dependencies in mdrun algorithms	Berk Hess	03/14/2018 08:47 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	
2462	GROMACS	Task	New	Normal	consider adding STL misuse tests		03/23/2018 01:23 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	
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	
2513	GROMACS	Bug	Feedback wanted	Normal	ref_t and temperature incorrect with coulomb-type = user	Yu Du	05/31/2018 04:05 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	
2532	GROMACS	Task	New	Normal	enable queue priorities in OpenCL		05/29/2018 02:29 PM	

#	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	
2538	GROMACS	Task	New	Normal	organize more of the PME GPU code along task-specific lines	Mark Abraham	05/31/2018 05:41 PM	
2556	GROMACS	Feature	New	Normal	make default selections suitable for DNA and RNA	Mark Abraham	06/20/2018 01:48 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	
2576	GROMACS	Bug	New	Normal	gmx potential -correct outputs the wrong potential		07/25/2018 02:58 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	
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	
2596	GROMACS	Feature	New	Normal	Constant potential method	Benson Muite	05/10/2019 09:54 AM	
2606	GROMACS	Bug	New	Normal	Free Energy Calculation -- Function type Fourier Dih. Not implemented in ip_pert		08/10/2018 01:48 AM	
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	Fix uploaded	Normal	GMXRC removes trailing colon from existing MANPATH		08/28/2018 03:13 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	
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	
2733	GROMACS	Bug	Blocked, need info	Normal	MdrunUtilityMpiUnitTests timesout on i686 and armv7hl with OpenMPI 2.1.5	Paul Bauer	01/17/2020 08:40 AM	
2739	GROMACS	Feature	New	Normal	Parallel continuous tempering and enhanced sampling feature		11/13/2018 11:36 PM	
2740	GROMACS	Bug	New	Normal	mdrun reports incorrect error with -bonded gpu without gpu	Mark Abraham	11/07/2018 01:59 PM	

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
2754	GROMACS	Bug	New	Normal	Simulated Tempering seems to be broken	Michael Shirts	02/05/2019 03:58 PM	
2762	GROMACS	Bug	Blocked, need info	Normal	incorrect results with Ubuntu 18.04 / glibc 2.27 (?) and >20 threads		07/01/2019 11:26 PM	
2764	GROMACS	Task	New	Normal	gmxapi version updates for post release-2019	Eric Irrgang	11/21/2018 12:53 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	
2818	GROMACS	Task	In Progress	Normal	bonded GPU kernel fusion	Magnus Lundborg	07/03/2019 09:01 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	
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	
2850	GROMACS	Task	In Progress	Normal	assess Raptor Talos for testing	Szilárd Páll	02/12/2019 01:14 PM	
2853	GROMACS	Bug	New	Normal	EwaldUnitTests segfault on armv7hl with gcc-9.0.1	Paul Bauer	02/04/2019 05:34 PM	
2854	GROMACS	Bug	New	Normal	OnlineHelpUnitTests segfaults on s390x with gcc-9.0.1	Paul Bauer	02/04/2019 11:17 AM	
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	
2864	GROMACS	Task	New	Normal	Building incompatibilities	Benson Muite	02/19/2019 02:00 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	
2874	GROMACS	Task	New	Normal	Refactor Gromacs (cluster) neighborlist into separate module	Erik Lindahl	02/28/2019 11:36 AM	
2876	GROMACS	Bug	New	Normal	2019.1 make check fails on AVX and AVX2 (Intel 2018u3)	Erik Lindahl	03/08/2019 10:32 AM	
2882	GROMACS	Task	New	Normal	evaluate different storage layouts for GPU coordinates/changes/forces	Szilárd Páll	03/07/2019 06:21 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	

#	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	
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	
2908	GROMACS	Task	New	Normal	Renaming things in nbxnm	Berk Hess	03/28/2019 10:10 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	
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	
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 opencl 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	
2984	GROMACS	Feature	New	Normal	More Extensive Selections Examples	Dallas Warren	06/18/2019 11:50 PM	
2993	GROMACS	Feature	New	Normal	Scalar and structured type expression and definitions for API	Eric Irrgang	10/17/2019 09:55 AM	
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	

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
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	
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	
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	
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	
3068	GROMACS	Bug	New	Normal	Misleading warning on rerun		08/26/2019 03:44 PM	
3073	GROMACS	Bug	New	Normal	Total potential energy goes crazy, but I don't know why this happens.		09/04/2019 07:25 PM	
3075	GROMACS	Bug	New	Normal	Frozen atoms are moving	Erik Lindahl	12/27/2019 10:51 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	
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	
3101	GROMACS	Bug	Blocked, need info	Normal	detect compilation failed	Erik Lindahl	12/27/2019 10:52 AM	
3115	GROMACS	Feature	New	Normal	Device stream manager		10/04/2019 09:00 AM	
3116	GROMACS	Bug	New	Normal	regressiontests/freeenergy core dumps on ppc64le	Paul Bauer	10/04/2019 10:52 PM	
3123	GROMACS	Task	New	Normal	address sanitizer coverage of parallelization code-paths		10/05/2019 12:32 AM	

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
3126	GROMACS	Feature	New	Normal	State propagator GPU data manager		10/09/2019 02:42 PM	
3127	GROMACS	Bug	New	Normal	mddrun-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	
3134	GROMACS	Feature	Feedback wanted	Normal	gmxapi Python exception names may need improvement	Eric Irrgang	10/13/2019 01:50 PM	
3135	GROMACS	Feature	New	Normal	Make GPU traits into 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	
3139	GROMACS	Task	New	Normal	gmxapi Futures should be subscribable	Eric Irrgang	10/15/2019 03:56 PM	
3149	GROMACS	Feature	New	Normal	Python user interface for obtaining simulation artifacts as files.	Eric Irrgang	10/15/2019 06:21 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	
3179	GROMACS	Feature	New	Normal	Clarify access to parallel data outputs	Eric Irrgang	10/26/2019 12:23 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	

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