

Issues

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
2513	GROMACS	Bug	Feedback wanted	Normal	ref_t and temperature incorrect with coulomb-type = user	Yu Du	05/31/2018 04:05 PM	
2601	GROMACS	Feature	New	Normal	Free energy calculations, soft-core potential	Vytautas Gapsys	02/10/2020 11:29 AM	future
2546	GROMACS	Task	New	Normal	Add more assertions to AWH code	Viveca Lindahl	06/06/2018 11:20 AM	future
2547	GROMACS	Feature	New	Low	Add option of averaging and obtaining error bars for AWH PMFs	Viveca Lindahl	06/06/2018 11:31 AM	future
2491	GROMACS	Feature	New	Low	Allow constant bias AWH simulations	Viveca Lindahl	06/05/2018 10:38 PM	future
2224	GROMACS	Feature	New	Normal	Proposed feature: conditional stop	Vedran Miletic	12/20/2019 12:11 PM	2021
3050	GROMACS	Bug	New	Low	Fix tests on Solaris	Vedran Miletic	02/27/2020 11:05 AM	2020.2
3368	GROMACS	Bug	New	Normal	Erroneous interplay between gmx rms command and atommass.dat: Can not find mass in database for atom MG in residue	Vedat Durmaz	02/05/2020 04:51 PM	future
2791	GROMACS	Feature	In Progress	Normal	Implement a module for lambda-dynamics simulations (lambda_site module)	Thomas Ullmann	03/01/2019 01:36 AM	future
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	
1010	GROMACS	Task	In Progress	Normal	Better support for multiple AnalysisData datasets	Teemu Murtola	07/11/2016 08:23 PM	
3415	GROMACS	Task	New	Normal	Port Pre-submit matrix to Gitlab CI	Szilárd Páll	03/23/2020 10:09 AM	2021-refactoring
2660	GROMACS	Task	New	Low	rework OpenCL nbnxn kernel constants	Szilárd Páll	12/28/2019 10:53 AM	future
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
1943	GROMACS	Task	Accepted	Low	make sure releases are submitted early for Debian Experimental	Szilárd Páll	12/20/2019 12:05 PM	2021
1826	GROMACS	Task	New	Normal	investigate non-optimal results with CPU-GPU balancing on AMD	Szilárd Páll	12/20/2019 12:04 PM	future
3216	GROMACS	Task	New	Normal	improve CPU force reductions	Szilárd Páll	12/04/2019 09:24 PM	
2882	GROMACS	Task	New	Normal	evaluate different storage layouts for GPU coordinates/changes/forces	Szilárd Páll	03/07/2019 06:21 PM	
2850	GROMACS	Task	In Progress	Normal	assess Raptor Talos for testing	Szilárd Páll	02/12/2019 01:14 PM	
2696	GROMACS	Task	In Progress	Normal	ensure PME queue is flushed	Szilárd Páll	12/31/2018 11:21 AM	future
2379	GROMACS	Task	New	Normal	check leftover FIXMEs in r2018	Szilárd Páll	12/31/2018 11:16 AM	future
2490	GROMACS	Task	New	Normal	evaluate two-step communicators	Szilárd Páll	10/03/2018 09:47 PM	future
1515	GROMACS	Task	New	Normal	improve g_bar output	Szilárd Páll	07/11/2016 08:10 PM	

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
1456	GROMACS	Task	New	Low	remove the use of nbat->alloc/free pointers	Szilárd Páll	06/20/2015 11:53 PM	
1211	GROMACS	Task	New	Low	improve use of preprocessor macros in CUDA kernels	Szilárd Páll	01/12/2015 06:42 PM	future
1464	GROMACS	Feature	New	Normal	implement PP-PME re-balancing	Szilárd Páll	10/16/2015 08:34 AM	future
3071	GROMACS	Bug	Accepted	Normal	complex.nbxn-ljpmc-LB-geometric failing with OpenCL timing debug mode assertions	Szilárd Páll	02/25/2020 03:39 PM	2020.2
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	
3266	GROMACS	Bug	New	High	gmx density show wrong symmetrize density profile using -symm?	Super duper	02/28/2020 08:24 AM	2020.2
948	GROMACS	Task	New	Normal	C++ thread synchronization primitives	Sander Pronk	07/11/2016 08:24 PM	
629	Support Platforms	Task	In Progress	Normal	List of users needs cleanup	Rossen Apostolov	02/21/2018 02:07 PM	
694	Support Platforms	Feature	Feedback wanted	Normal	Write instructions/policy for issue handling	Rossen Apostolov	05/31/2017 05:41 PM	
1030	GROMACS	Feature	Fix uploaded	Low	adding -tu option to some analysis tools	Rossen Apostolov	07/11/2016 08:22 PM	
996	GROMACS	Task	New	Normal	C++ MPI Framework	Roland Schulz	07/14/2014 11:53 AM	future
2595	GROMACS	Task	New	Normal	Reusable Utilities for Schedules	Prashanth Kanduri	02/22/2019 03:48 PM	future
2621	GROMACS	Task	New	Normal	Fine-Grained API to Describe Force Calculation and Neighbourhood Search	Prashanth Kanduri	08/22/2018 11:36 AM	future
2574	GROMACS	Feature	New	Normal	iForceSchedule Abstraction	Prashanth Kanduri	03/29/2019 05:20 PM	future
2594	GROMACS	Feature	New	Normal	Multi-level GMX API	Prashanth Kanduri	02/22/2019 03:48 PM	future
2045	GROMACS	Task	New	Normal	API design and language bindings	Peter Kasson	01/29/2020 03:59 PM	
1786	GROMACS	Task	New	Normal	Python style standards in developer docs	Peter Kasson	12/26/2019 03:15 PM	
3275	GROMACS	Task	New	Normal	Document Gitlab CI instead of Jenkins and releng	Paul Bauer	03/09/2020 05:55 PM	2021-infrastructure-stable
3331	GROMACS	Task	New	Low	Run physical validation tests in Gitlab	Paul Bauer	02/27/2020 11:09 PM	future
3272	GROMACS	Task	New	Normal	Port complete CI testing to Gitlab	Paul Bauer	02/27/2020 11:04 AM	2021-infrastructure-stable
3361	GROMACS	Task	New	Normal	Gitlab source archive contains files from build directory	Paul Bauer	02/25/2020 10:13 AM	2020.2
3264	GROMACS	Task	New	Normal	Break up MdrunMpiTests	Paul Bauer	12/23/2019 11:44 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
2833	GROMACS	Task	New	Normal	Update topology datastructures	Paul Bauer	12/02/2019 01:43 PM	2021-infrastructure-stable
2396	GROMACS	Task	New	Normal	Refactor trajectoryanalysis module to allow handling of trajectory frame manipulation	Paul Bauer	12/02/2019 01:24 PM	2021-infrastructure-stable
2916	GROMACS	Task	New	Normal	Decide future of symtab	Paul Bauer	09/06/2019 02:35 PM	2021-infrastructure-stable

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
3035	GROMACS	Task	New	Normal	Provide central logger in wrapper binary	Paul Bauer	09/06/2019 02:34 PM	2021-infrastructure-stable
2603	GROMACS	Task	New	Normal	Add ability to properly check coordinate files during testing	Paul Bauer	10/15/2018 01:16 PM	future
2383	GROMACS	Task	New	Normal	Add JSON interface to write and read files	Paul Bauer	01/16/2018 02:01 PM	future
3294	GROMACS	Bug	New	Normal	multiple tests fail on fedora 31	Paul Bauer	02/28/2020 03:12 PM	2020.2
3333	GROMACS	Bug	New	Normal	Assertion failure when trying to get unit test help	Paul Bauer	02/25/2020 10:16 AM	2021-infrastructure-stable
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	
3116	GROMACS	Bug	New	Normal	regressiontests/freenenergy core dumps on ppc64le	Paul Bauer	10/04/2019 10:52 PM	
3113	GROMACS	Bug	New	Low	Use of read_tps_conf is depeccated	Paul Bauer	10/01/2019 11:36 AM	2021-infrastructure-stable
2734	GROMACS	Bug	In Progress	Normal	regressiontests/kernel core dumps on ppc64le	Paul Bauer	06/15/2019 04:12 PM	future
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	
2483	GROMACS	Bug	New	Low	gmx dump writes mdp files that can not be parsed by grompp	Paul Bauer	10/08/2018 10:50 AM	future
3422	GROMACS	Task	Resolved	Normal	Implement modular checkpointing for modular simulator	Pascal Merz	09/16/2020 09:45 AM	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
3421	GROMACS	Task	New	Normal	Implement client system for global reduction	Pascal Merz	03/11/2020 03:31 PM	2021-infrastructure-stable
3437	GROMACS	Task	New	Normal	Use builders to prepare modules	Pascal Merz	03/11/2020 07:05 AM	2021-infrastructure-stable
3419	GROMACS	Task	New	Normal	Reduce / remove use of legacy t_state objects throughout modular simulator	Pascal Merz	03/10/2020 10:24 PM	2021-infrastructure-stable
3418	GROMACS	Task	New	Normal	Infrastructure improvements for modular simulator	Pascal Merz	03/10/2020 10:24 PM	2021-infrastructure-stable
3420	GROMACS	Task	New	Normal	Unify force and shellfc elements for modular simulator	Pascal Merz	03/10/2020 09:50 PM	2021-infrastructure-stable
3417	GROMACS	Feature	New	Normal	Make modular simulator feature-complete	Pascal Merz	03/23/2020 03:57 AM	2021-infrastructure-stable
3426	GROMACS	Feature	New	Normal	Support acceleration in modular simulator	Pascal Merz	03/11/2020 04:09 PM	2021-infrastructure-stable
3433	GROMACS	Feature	New	Normal	Decide how to handle multisim with modular simulator	Pascal Merz	03/11/2020 06:42 AM	2021-infrastructure-stable
3436	GROMACS	Feature	New	Normal	Implement AWH for modular simulator	Pascal Merz	03/11/2020 06:32 AM	2021-infrastructure-stable
3435	GROMACS	Feature	New	Normal	Implement pull for modular simulator	Pascal Merz	03/11/2020 06:31 AM	2021-infrastructure-stable
3434	GROMACS	Feature	New	Normal	Support box deformation in modular simulator	Pascal Merz	03/11/2020 12:50 AM	2021-infrastructure-stable
3432	GROMACS	Feature	New	Normal	Implement essential dynamics for modular simulator	Pascal Merz	03/11/2020 12:38 AM	2021-infrastructure-stable
3431	GROMACS	Feature	New	Normal	Implement virtual sites for modular simulator	Pascal Merz	03/11/2020 12:33 AM	2021-infrastructure-stable
3430	GROMACS	Feature	New	Normal	Implement NMR restraints for modular simulator	Pascal Merz	03/11/2020 12:28 AM	2021-infrastructure-stable
3428	GROMACS	Feature	New	Normal	Implement SIMD version of modular simulator propagators	Pascal Merz	03/11/2020 12:12 AM	2021-infrastructure-stable
3427	GROMACS	Feature	New	Normal	Support freeze groups in modular simulator	Pascal Merz	03/11/2020 12:07 AM	2021-infrastructure-stable
3425	GROMACS	Feature	New	Normal	Implement rerun for the modular simulator	Pascal Merz	03/10/2020 11:57 PM	2021-infrastructure-stable

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
3424	GROMACS	Feature	New	Normal	Implement stochastic dynamics / langevin integrator in modular simulator	Pascal Merz	03/10/2020 11:48 PM	2021-infrastructure-stable
3423	GROMACS	Feature	New	Normal	Implement additional temperature and pressure control algorithms for modular simulator	Pascal Merz	03/10/2020 11:22 PM	2021-infrastructure-stable
3363	GROMACS	Feature	New	Normal	Improve FEP testing	Pascal Merz	03/01/2020 03:22 PM	2021-infrastructure-stable
1509	GROMACS	Task	New	Low	Reduce the distance dependence of shifted potentials for free energies if possible	Michael Shirts	07/11/2016 08:10 PM	
1246	GROMACS	Task	New	Normal	expanded ensemble .tpr cannot be rerun	Michael Shirts	06/19/2015 01:56 PM	
2070	GROMACS	Feature	In Progress	Normal	Physical validation testing	Michael Shirts	01/03/2020 09:36 PM	future
2944	GROMACS	Feature	New	Normal	Roadmap for thermostats / barostats in new propagation/integration scheme	Michael Shirts	12/27/2019 04:00 PM	2021
2186	GROMACS	Feature	New	Low	Potential change for logical improvements: move control of constraints purely to the .mdp	Michael Shirts	11/27/2018 11:27 AM	future
1332	GROMACS	Feature	In Progress	Normal	Supporting multiple end states instead of just A and B	Michael Shirts	06/05/2018 03:58 PM	
1652	GROMACS	Feature	New	Normal	Decide how to represent multiple lambda states internally	Michael Shirts	06/05/2018 03:58 PM	
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	
2137	GROMACS	Feature	New	Normal	Preliminary refactoring of constraints and update machinery.	Michael Shirts	03/11/2017 08:32 AM	future
1137	GROMACS	Feature	New	Normal	Proposal for integrator framework (do_md) in future GROMACS	Michael Shirts	02/21/2017 12:48 AM	future
1303	GROMACS	Feature	New	Normal	Adding lambda dependent distance for pull code	Michael Shirts	07/11/2016 08:18 PM	
1562	GROMACS	Feature	New	Normal	introducing a Monte Carlo framework (first application: MC barostat)	Michael Shirts	07/11/2016 08:08 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	
1335	GROMACS	Feature	New	Normal	Improved interaction of free energies with pull code to better support Hamiltonian replica exchange with umbrella sampling	Michael Shirts	05/13/2014 10:38 AM	future
1142	GROMACS	Feature	New	Low	Synchronizing the differences between point estimation and histogram estimation for free energies	Michael Shirts	02/20/2014 08:27 PM	future
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
2754	GROMACS	Bug	New	Normal	Simulated Tempering seems to be broken	Michael Shirts	02/05/2019 03:58 PM	
1442	GROMACS	Bug	Feedback wanted	Normal	Not consistent solvation free energies differencies	Michael Shirts	07/11/2016 08:13 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	
1339	GROMACS	Bug	New	Normal	Center of mass drift with Nose-Hoover, MTTK and md-vv	Michael Shirts	06/18/2015 08:53 PM	future
2495	GROMACS	Task	Accepted	Normal	replace -noconfout with mdp option	Mark Abraham	12/28/2019 10:39 AM	2021

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
2889	GROMACS	Task	New	Normal	update grompp warnings for brevity, usefulness and actionability	Mark Abraham	12/27/2019 04:38 PM	future
2877	GROMACS	Task	New	Normal	use gmx::Options more	Mark Abraham	12/20/2019 01:22 PM	2021
2425	GROMACS	Task	New	Normal	testing multisim with multiple ranks per simulation	Mark Abraham	12/20/2019 12:13 PM	2021
1781	GROMACS	Task	Accepted	Normal	re-design benchmarking functionality	Mark Abraham	12/20/2019 12:03 PM	future
3131	GROMACS	Task	New	Normal	support ccache with clang-tidy	Mark Abraham	12/20/2019 08:20 AM	2021-infrastructure-stable
2395	GROMACS	Task	In Progress	Normal	break up commrec	Mark Abraham	12/15/2019 11:51 AM	2021-infrastructure-stable
1505	GROMACS	Task	New	Normal	improve handling of logging	Mark Abraham	01/02/2019 06:06 PM	
1793	GROMACS	Task	New	Normal	cleanup of integration loop	Mark Abraham	10/31/2018 10:49 PM	future
1937	GROMACS	Task	New	Low	stop supporting changing CUDA host compiler	Mark Abraham	10/15/2018 05:19 PM	future
2644	GROMACS	Task	New	Normal	Replace compute_globals	Mark Abraham	09/24/2018 05:51 PM	future
2492	GROMACS	Task	New	Normal	implement force calculation via ForceProviders containing collections of IForceProvider	Mark Abraham	09/19/2018 03:13 PM	future
2423	GROMACS	Task	New	Normal	modernize constraints code	Mark Abraham	09/19/2018 03:01 PM	future
2538	GROMACS	Task	New	Normal	organize more of the PME GPU code along task-specific lines	Mark Abraham	05/31/2018 05:41 PM	
1411	GROMACS	Task	New	Normal	Future of thread_mpi	Mark Abraham	02/26/2018 04:56 PM	future
1963	GROMACS	Task	New	Low	collect examples of systems where users tried to do something that performed badly	Mark Abraham	08/09/2016 07:30 AM	
1056	GROMACS	Task	Accepted	Normal	status of fft5d_threads and fftw3_threads functionality	Mark Abraham	07/11/2016 08:21 PM	
1947	GROMACS	Task	New	Normal	Consider fixing corner case in TinyXML2	Mark Abraham	04/19/2016 01:40 AM	
1758	GROMACS	Task	New	Normal	Verlet scheme reorganization / modularization	Mark Abraham	07/20/2015 06:33 PM	future
1490	GROMACS	Task	New	Normal	Usage of forward declarations vs typedef vs #include	Mark Abraham	01/21/2015 10:23 AM	
1373	GROMACS	Task	New	Low	Add missing nbxn tests	Mark Abraham	06/09/2014 08:36 PM	
765	GROMACS	Task	New	Normal	Improving serialization of data structures prior to communication	Mark Abraham	05/13/2014 10:04 AM	future
1214	GROMACS	Task	New	Normal	Keep track of important changes for Changelog	Mark Abraham	06/26/2013 11:24 AM	
1500	GROMACS	Feature	New	Normal	Post-5.0 feature clean-up plan	Mark Abraham	08/26/2019 03:47 PM	
2229	GROMACS	Feature	New	High	Full Object Oriented Modularization of GROMACS MDRUN Codebase	Mark Abraham	08/22/2018 05:03 PM	future
2556	GROMACS	Feature	New	Normal	make default selections suitable for DNA and RNA	Mark Abraham	06/20/2018 01:48 PM	
2090	GROMACS	Feature	New	Normal	redirecting stdout or stderr for testing	Mark Abraham	12/15/2016 03:15 AM	
1397	GROMACS	Feature	New	Normal	gmx eneconv -offset 1.998 -dt 2 is broken for large times	Mark Abraham	06/12/2014 01:31 AM	future
1247	GROMACS	Feature	New	Normal	fix hardcoded references to atom names in analysis tools	Mark Abraham	06/12/2014 01:20 AM	future
1518	GROMACS	Feature	New	Low	Enable automatic build checking for newer versions	Mark Abraham	06/04/2014 04:13 PM	future
2832	GROMACS	Bug	New	Low	PaddedVector move operations broken	Mark Abraham	12/28/2019 10:40 AM	2021
2480	GROMACS	Bug	New	Normal	pdb2gmx does not protonate correctly for united-atom Gromos	Mark Abraham	12/20/2019 12:17 PM	2021

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
2740	GROMACS	Bug	New	Normal	mdrun reports incorrect error with -bonded gpu without gpu	Mark Abraham	11/07/2018 01:59 PM	
2020	GROMACS	Bug	New	Normal	Possible issue with md-vv integrator	Mark Abraham	03/11/2017 08:30 AM	
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	
1190	GROMACS	Bug	New	Normal	Use of FORCE in setting cached variables	Mark Abraham	06/17/2014 06:09 AM	
2818	GROMACS	Task	In Progress	Normal	bonded GPU kernel fusion	Magnus Lundborg	07/03/2019 09:01 PM	
3117	GROMACS	Feature	New	Normal	Coulomb FEP PME on GPU	Magnus Lundborg	02/17/2020 03:58 PM	2021-infrastructure-stable
3371	GROMACS	Feature	New	Normal	Control FEP using AWH	Magnus Lundborg	02/06/2020 02:20 PM	2021
2188	TNG trajectory library	Feature	Resolved	High	Masses missing from TNG specification	Magnus Lundborg	06/13/2017 05:08 PM	
1864	GROMACS	Feature	New	Normal	write tng files with energies	Magnus Lundborg	07/11/2016 08:00 PM	
1229	TNG trajectory library	Feature	Resolved	Normal	Selection groups	Magnus Lundborg	11/29/2013 04:38 PM	version 1
1367	TNG trajectory library	Feature	In Progress	Normal	Break tng_io.c into smaller files	Magnus Lundborg	10/25/2013 10:49 AM	version 1
1198	TNG trajectory library	Feature	In Progress	Normal	Full documentation for the high-level API	Magnus Lundborg	06/25/2013 10:05 PM	version 2
1199	TNG trajectory library	Feature	New	Normal	residue numbering	Magnus Lundborg	04/24/2013 09:33 AM	version 2
1200	TNG trajectory library	Feature	New	Normal	Field for the PDB format 'segment identifier'	Magnus Lundborg	04/24/2013 09:32 AM	version 2
1252	TNG trajectory library	Bug	Feedback wanted	Normal	residual ids and atomIDs	Magnus Lundborg	06/12/2013 10:35 AM	version 1
2766	GROMACS	Task	In Progress	Normal	Improve hardware option selection	Kevin Boyd	12/20/2019 02:34 PM	2021
2368	GROMACS	Task	In Progress	Normal	update implementation of gmx msd	Kevin Boyd	11/03/2018 07:43 PM	future
2501	GROMACS	Task	New	Normal	Documentation section on log file contents	Kevin Boyd	10/03/2018 09:48 PM	future
868	GROMACS	Feature	In Progress	Normal	Implement parallelization support to analysis framework	Kevin Boyd	12/20/2019 11:59 AM	2021
3446	GROMACS	Task	New	Normal	apply maintainability updates across all GPU kernels	Jonathan Vincent	03/19/2020 03:31 PM	
3445	GROMACS	Task	New	Normal	create heuristic for c_skipNeutralAtoms	Jonathan Vincent	03/17/2020 12:12 PM	
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

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
3355	GROMACS	Feature	Accepted	Normal	New PME parallel (GPU) scheme	Jonathan Vincent	02/12/2020 11:58 AM	
3416	GROMACS	Task	New	Normal	Port post-submit matrix to Gitlab CI	Joe Jordan	03/16/2020 05:50 PM	2021-refactoring
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
2735	GROMACS	Task	New	Normal	Allow gmx_genrestr to write correct position restraints for molecules after the first molecule	Joe Jordan	12/11/2019 09:26 AM	future
2442	GROMACS	Task	New	Normal	Port gmx saxs and gmx sans to c++	Joe Jordan	06/28/2018 10:06 PM	future
2874	GROMACS	Task	New	Normal	Refactor Gromacs (cluster) neighborlist into separate module	Erik Lindahl	02/28/2019 11:36 AM	
2216	GROMACS	Task	New	Normal	GROMACS SIMD acceleration: generation 3	Erik Lindahl	07/17/2017 06:57 PM	future
1168	GROMACS	Feature	In Progress	Low	g_density does not do what users think it does, given PBC over z and constant pressure simulation	Erik Lindahl	10/20/2018 12:49 AM	future
1666	GROMACS	Feature	New	Normal	new approach for Verlet-scheme kernel generation	Erik Lindahl	10/08/2018 07:04 PM	future
843	GROMACS	Feature	New	Low	g_helixorient could benefit from more documentation	Erik Lindahl	05/23/2014 02:02 PM	
3380	GROMACS	Bug	Resolved	Low	IBM VSX checks fail with gcc-10	Erik Lindahl	04/30/2020 01:30 PM	2020.2
3249	GROMACS	Bug	In Progress	Low	cmake bad tests for avx512 on AMD	Erik Lindahl	02/26/2020 05:00 PM	
3265	GROMACS	Bug	Blocked, need info	Low	regressiontests/complex fails on ppc64le	Erik Lindahl	01/09/2020 05:00 PM	
3101	GROMACS	Bug	Blocked, need info	Normal	detect compilation failed	Erik Lindahl	12/27/2019 10:52 AM	
3075	GROMACS	Bug	New	Normal	Frozen atoms are moving	Erik Lindahl	12/27/2019 10:51 AM	
3234	GROMACS	Bug	Accepted	Normal	Signal: Floating point exception Signal code: Floating point divide-by-zero	Erik Lindahl	12/16/2019 03:40 PM	
2876	GROMACS	Bug	New	Normal	2019.1 make check fails on AVX and AVX2 (Intel 2018u3)	Erik Lindahl	03/08/2019 10:32 AM	
1618	GROMACS	Bug	In Progress	Normal	g_protonate segfaults unconditionally	Erik Lindahl	08/17/2015 02:10 PM	
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
3289	GROMACS	Task	New	Normal	Distinguish identifying and non-identifying inputs to API operations.	Eric Irrgang	01/10/2020 11:30 AM	
3130	GROMACS	Task	New	Normal	Interim handling of gmxapi data references.	Eric Irrgang	12/11/2019 11:26 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
3174	GROMACS	Task	Feedback wanted	Low	Proposed gmxapi syntax update: "input" and "output" key word arguments -> "inputs" and "outputs"	Eric Irrgang	10/23/2019 06:34 PM	
3139	GROMACS	Task	New	Normal	gmxapi Futures should be subscribable	Eric Irrgang	10/15/2019 03:56 PM	
2764	GROMACS	Task	New	Normal	gmxapi version updates for post release-2019	Eric Irrgang	11/21/2018 12:53 PM	
3393	GROMACS	Feature	Resolved	Normal	Allow gmxapi.commandline_operation to use STDIN	Eric Irrgang	02/25/2020 05:15 PM	2021-infrastructure-stable

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
3394	GROMACS	Feature	New	Normal	improve gmxapi error handling	Eric Irrgang	02/24/2020 11:45 AM	2021-infrastructure-stable
3295	GROMACS	Feature	New	Normal	Expand gmxapi.modify_input use cases.	Eric Irrgang	01/16/2020 05:13 PM	2021-refactoring
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
3038	GROMACS	Feature	New	Normal	Improvements to MD plugin development environment	Eric Irrgang	12/10/2019 01:58 PM	2021-infrastructure-stable
2996	GROMACS	Feature	In Progress	Normal	gmxapi execution model	Eric Irrgang	12/10/2019 01:57 PM	2021-infrastructure-stable
3179	GROMACS	Feature	New	Normal	Clarify access to parallel data outputs	Eric Irrgang	10/26/2019 12:23 PM	
2993	GROMACS	Feature	New	Normal	Scalar and structured type expression and definitions for API	Eric Irrgang	10/17/2019 09:55 AM	
3148	GROMACS	Feature	New	Normal	Roadmap for gmxapi filesystem interactions.	Eric Irrgang	10/15/2019 06:23 PM	2021-infrastructure-stable
3149	GROMACS	Feature	New	Normal	Python user interface for obtaining simulation artifacts as files.	Eric Irrgang	10/15/2019 06:21 PM	
3147	GROMACS	Feature	New	Normal	gmxapi workflow checkpointing	Eric Irrgang	10/15/2019 06:18 PM	2021-infrastructure-stable
3134	GROMACS	Feature	Feedback wanted	Normal	gmxapi Python exception names may need improvement	Eric Irrgang	10/13/2019 01:50 PM	
3408	GROMACS	Bug	Fix uploaded	Normal	Gmxapi* tests segfault in rpmbuild	Eric Irrgang	03/23/2020 01:27 PM	2020.2
3136	GROMACS	Bug	New	Normal	gmxapi.operation data flow topology unclear or incomplete	Eric Irrgang	12/11/2019 11:25 AM	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
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
3150	GROMACS	Bug	New	Normal	gmxapi data type annotations are confusing and inadequate	Eric Irrgang	10/22/2019 03:08 PM	2021-infrastructure-stable
3172	GROMACS	Feature	New	Normal	QM/MM Interface with CP2K	Dmitry Morozov	01/17/2020 12:18 PM	future
1323	GROMACS	Task	New	Normal	determine future of existing tools for	David van der Spoel	12/04/2018 11:53 AM	
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
2774	GROMACS	Feature	New	Normal	Refactor shell code into its own integrator	David van der Spoel	12/27/2019 04:05 PM	2021
2451	GROMACS	Feature	Resolved	Normal	Linear virtual sites with fixed distance	David van der Spoel	09/16/2019 01:15 PM	
2034	GROMACS	Feature	New	Normal	Unit tests for bonded forces	David van der Spoel	06/29/2019 10:22 AM	future
2866	GROMACS	Feature	New	Normal	Alternative non-bonded potentials	David van der Spoel	03/05/2019 03:50 PM	future
2545	GROMACS	Feature	New	Normal	Should grompp fix periodicity of input files?	David van der Spoel	10/03/2018 11:32 PM	future
1498	GROMACS	Feature	New	Low	g_dipoles does not work properly with ionic systems	David van der Spoel	07/11/2016 08:11 PM	

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
1377	GROMACS	Feature	Feedback wanted	Low	Replica exchange if replicas not in ascendent T	David van der Spoel	06/23/2016 03:48 PM	
1167	GROMACS	Feature	New	Low	trjconv -center would be more intuitive if it centered the center of mass, not the midpoint between minimum and maximum values	David van der Spoel	06/23/2014 04:13 AM	future
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	
1166	GROMACS	Bug	New	Low	g_order is incorrect for unsaturated carbons	David van der Spoel	02/06/2020 02:32 PM	future
3049	GROMACS	Bug	New	Low	gmx nmeig should plot a real infrared spectrum	David van der Spoel	09/24/2019 03:25 PM	future
1354	GROMACS	Bug	New	Normal	Constant acceleration NEMD is broken.	David van der Spoel	01/09/2019 04:42 PM	
2544	GROMACS	Bug	New	Normal	gmx rmsf does not fix periodicity in reference structure	David van der Spoel	08/21/2018 10:36 AM	future
2052	GROMACS	Bug	New	Low	trjconv does not recognize periodic molecules	David van der Spoel	01/12/2018 11:05 AM	
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	
1235	GROMACS	Bug	New	Normal	peptide dihedral angle definitions violate IUPAC	David van der Spoel	06/19/2015 12:24 AM	future
1481	GROMACS	Bug	New	Low	g_chi output file chi.log reports atomic definitions for phi and psi that do not correspond to the angles output in the .xvg files	David van der Spoel	06/12/2014 01:37 PM	
2984	GROMACS	Feature	New	Normal	More Extensive Selections Examples	Dallas Warren	06/18/2019 11:50 PM	
1849	GROMACS	Feature	New	Normal	expanded ensemble -- Adaptive Integration Method	Christopher Mirabzadeh	07/11/2016 08:01 PM	
3306	GROMACS	Task	New	Normal	Document gmx dos tool more clearly	Christian Blau	01/20/2020 02:31 PM	future
3076	GROMACS	Task	New	Normal	Selectively activate MdModules during simulation instead of instantiating all of them	Christian Blau	01/17/2020 02:40 PM	2021-infrastructure-stable
2834	GROMACS	Task	In Progress	Normal	C++ matrix classes	Christian Blau	12/29/2019 10:32 AM	2021
3260	GROMACS	Task	New	Low	keep up to with mdspan reference implementation	Christian Blau	12/20/2019 01:16 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
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
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
3072	GROMACS	Task	New	Normal	Use gmx::index for indexing instead of int	Christian Blau	09/03/2019 04:23 PM	2021-infrastructure-stable
2658	GROMACS	Task	New	Normal	Secondary structure assignment via DSSP as native gromacs code	Christian Blau	10/09/2018 04:51 PM	future

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
2590	GROMACS	Task	New	Normal	Essential Dynamics as module providing forces	Christian Blau	08/22/2018 05:03 PM	future
2017	GROMACS	Task	In Progress	Normal	Modularize simulation option storage and reading from mdp files	Christian Blau	04/06/2018 06:07 PM	future
3069	GROMACS	Feature	New	Low	Iterator over span and indices into this span (zip-style iterator)	Christian Blau	08/29/2019 11:11 AM	future
2282	GROMACS	Feature	New	Normal	Density map toolset	Christian Blau	03/21/2019 06:08 PM	future
2005	GROMACS	Feature	New	Normal	Full Correlation Analysis (FCA) as Trajectory Analysis Module	Christian Blau	02/07/2018 02:19 PM	future
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
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
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	
3410	GROMACS	Feature	New	Normal	Random Acceleration Molecular Dynamics (RAMD)	Bernd Doser	03/05/2020 03:22 PM	2021
2283	GROMACS	Feature	New	Normal	Force distribution analysis	Bernd Doser	10/27/2017 11:44 AM	
2822	GROMACS	Task	Accepted	Normal	Make nbxn a module	Berk Hess	12/18/2019 10:49 AM	future
2875	GROMACS	Task	Accepted	Normal	SIMD version of the free-energy kernel	Berk Hess	12/02/2019 01:44 PM	2021-infrastructure-stable
2908	GROMACS	Task	New	Normal	Renaming things in nbxnm	Berk Hess	03/28/2019 10:10 AM	
2452	GROMACS	Task	In Progress	Normal	Reduce data dependencies in mdrun algorithms	Berk Hess	03/14/2018 08:47 PM	
2071	GROMACS	Task	In Progress	High	Low accuracy default settings yield incorrect liquid densities	Berk Hess	01/05/2018 03:32 PM	
2238	GROMACS	Task	In Progress	Normal	GPU emulation mode support for rolling pruning missing	Berk Hess	12/21/2017 03:21 PM	
1347	GROMACS	Feature	New	Normal	future of tables	Berk Hess	01/09/2020 02:37 PM	future
1192	GROMACS	Feature	Accepted	Normal	Add support for Verlet scheme with Buckingham	Berk Hess	07/11/2016 08:19 PM	
1658	GROMACS	Feature	New	Normal	Electrostatics treatment for multiple lambda sites	Berk Hess	07/11/2016 08:05 PM	
1162	GROMACS	Feature	New	Normal	Implement gb_saltconc	Berk Hess	02/26/2013 05:33 PM	future
1053	GROMACS	Feature	In Progress	Normal	L-BFGS doesn't use constraints or call do_em_step	Berk Hess	01/18/2013 11:00 AM	future
760	GROMACS	Feature	New	Low	Implement rigid body groups	Berk Hess	12/30/2012 06:04 AM	future
3441	GROMACS	Bug	Resolved	Normal	Ewald surface-epsilon is incorrect	Berk Hess	03/18/2020 11:15 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
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
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
1880	GROMACS	Bug	Feedback wanted	Normal	PP-PME load balancing issue	Berk Hess	10/03/2018 09:45 PM	future
1843	GROMACS	Bug	In Progress	Normal	pbx=xy with 2 walls floating point exception with the verlet scheme	Berk Hess	10/31/2016 11:35 AM	
2864	GROMACS	Task	New	Normal	Building incompatibilities	Benson Muite	02/19/2019 02:00 PM	

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
2596	GROMACS	Feature	New	Normal	Constant potential method	Benson Muite	05/10/2019 09:54 AM	
2755	GROMACS	Feature	New	Low	md5 sums and sha256, sha512 hashes	Benson Muite	02/19/2019 11:00 PM	
3317	GROMACS	Task	Resolved	Normal	Improve testing of the GPU code	Artem Zhmurov	10/06/2020 12:15 PM	2021-refactoring
3314	GROMACS	Task	Resolved	Normal	Platform agnostic DeviceStream	Artem Zhmurov	03/20/2020 09:55 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
3315	GROMACS	Task	Resolved	Normal	Platform agnostic DeviceContext	Artem Zhmurov	03/11/2020 04:15 PM	2021-refactoring
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
3348	GROMACS	Task	New	Normal	GPU LINCS and SETTLE: unify virial reduction	Artem Zhmurov	01/23/2020 11:58 AM	2021-infrastructure-stable
3346	GROMACS	Task	New	Normal	GPU SETTLE: Use the same parameters and parameters initialization in GPU and CPU versions of SETTLE.	Artem Zhmurov	01/23/2020 11:58 AM	2021-infrastructure-stable
3345	GROMACS	Task	New	Normal	GPU update-constraints: Reconsider the naming of coordinates buffer in constraints.	Artem Zhmurov	01/23/2020 11:57 AM	2021-infrastructure-stable
3344	GROMACS	Task	New	Normal	GPU update-constraints: Better virial reduction.	Artem Zhmurov	01/23/2020 11:57 AM	2021-infrastructure-stable
3343	GROMACS	Task	New	Normal	GPU SETTLE: Use different ordering for matrices.	Artem Zhmurov	01/23/2020 11:57 AM	2021-infrastructure-stable
3342	GROMACS	Task	New	Normal	GPU SETTLE: Read only one index per water molecule.	Artem Zhmurov	01/23/2020 11:56 AM	2021-infrastructure-stable
3341	GROMACS	Task	New	Normal	GPU LINCS: Use analytical solution for the matrix A inversion.	Artem Zhmurov	01/23/2020 11:56 AM	2021-infrastructure-stable
3340	GROMACS	Task	New	Normal	GPU LINCS: Move more data to local/shared memory	Artem Zhmurov	01/23/2020 11:56 AM	2021-infrastructure-stable
3339	GROMACS	Task	New	Normal	GPU LINCS: Warp-level synchronization for coupled constraints	Artem Zhmurov	01/23/2020 11:55 AM	2021-infrastructure-stable
3338	GROMACS	Task	New	Normal	GPU update-constraints: Do not save intermediate coordinates if there is no constraints	Artem Zhmurov	01/23/2020 11:55 AM	2021-infrastructure-stable
3337	GROMACS	Task	New	Normal	GPU update-constraints: Merge Leap-Frog, LINCS and SETTLE kernels.	Artem Zhmurov	01/23/2020 11:55 AM	2021-infrastructure-stable
3258	GROMACS	Task	New	Normal	GPU update-constraints: Enable free energy perturbation	Artem Zhmurov	01/23/2020 11:54 AM	2021-infrastructure-stable
3236	GROMACS	Task	New	Normal	GPU update-constraints: Pulling support	Artem Zhmurov	01/23/2020 11:53 AM	2021-infrastructure-stable
3162	GROMACS	Task	New	Normal	Add virtual site support to GPU version of update-constraints.	Artem Zhmurov	01/23/2020 11:52 AM	2021-infrastructure-stable
3323	GROMACS	Task	In Progress	Normal	Rework the StatePropagatorDataGpu	Artem Zhmurov	01/22/2020 09:50 AM	2021-refactoring
3322	GROMACS	Task	Accepted	Normal	Add reallocate(...) function that does not care about the contents of the buffer	Artem Zhmurov	01/22/2020 09:50 AM	2021-refactoring
3321	GROMACS	Task	Accepted	Normal	Add D2D wrapper	Artem Zhmurov	01/22/2020 09:50 AM	2021-refactoring
3320	GROMACS	Task	In Progress	Normal	Remove duplicating D2H/H2D wrappers in NBNXM	Artem Zhmurov	01/22/2020 09:50 AM	2021-refactoring
3319	GROMACS	Task	In Progress	Normal	Use DeviceBuffer instead of native GPU types in NBNXM	Artem Zhmurov	01/22/2020 09:49 AM	2021-refactoring
3316	GROMACS	Task	Accepted	Normal	Context and Stream manager	Artem Zhmurov	01/22/2020 09:49 AM	2021-refactoring
3155	GROMACS	Task	Accepted	Normal	Unify DD and CPU-GPU gather & scatter	Artem Zhmurov	10/17/2019 03:50 PM	2021-infrastructure-stable

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
3114	GROMACS	Feature	New	Normal	Improve GPU update-constraints module	Artem Zhmurov	02/10/2020 04:30 PM	2021
3318	GROMACS	Feature	In Progress	Normal	Use wrappers for the GPU buffer copy/allocations	Artem Zhmurov	01/23/2020 12:01 PM	2021-refactoring
3313	GROMACS	Feature	Accepted	Normal	Introduce and use opaque types for the DeviceStream and DeviceContext	Artem Zhmurov	01/23/2020 12:00 PM	2021-refactoring
3352	GROMACS	Feature	New	Normal	GPU update-constraints feature support	Artem Zhmurov	01/23/2020 11:59 AM	2021
3351	GROMACS	Feature	New	Normal	GPU update-constraints code organization and integration	Artem Zhmurov	01/23/2020 11:59 AM	2021
3350	GROMACS	Feature	New	Normal	GPU update-constraints performance	Artem Zhmurov	01/23/2020 11:59 AM	2021
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
438	GROMACS	Feature	In Progress	Low	New tool: g_correl	Alexey Shvetsov	06/20/2014 10:38 AM	future
2537	GROMACS	Task	New	Normal	Simplify PME solve reduction	Aleksei lupinov	12/20/2019 12:21 PM	future
2453	GROMACS	Task	Resolved	High	PME OpenCL porting effort	Aleksei lupinov	12/20/2019 12:18 PM	2021
2516	GROMACS	Task	New	Low	Support PME OpenCL execution width < 16	Aleksei lupinov	06/05/2019 05:32 PM	
2054	GROMACS	Feature	Accepted	High	PME on GPU	Aleksei lupinov	12/20/2019 12:18 PM	future
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
2859	GROMACS	Task	Resolved	Normal	Change ArrayRef iterator type from pointer to std::iterator		06/26/2020 06:15 PM	
3041	GROMACS	Task	Resolved	Normal	Remove workaround for gcc bug 58265		06/19/2020 04:45 PM	
3297	GROMACS	Task	Resolved	Normal	Require gcc > 5		04/30/2020 11:00 AM	2021-infrastructure-stable
2998	GROMACS	Task	Resolved	Normal	Update Python detection		04/23/2020 04:45 PM	2021-infrastructure-stable
3290	GROMACS	Task	Resolved	Normal	Require CMake >= 3.12		04/14/2020 02:45 PM	2021-refactoring
3271	GROMACS	Task	Resolved	Normal	Adopt PEP-518 for Python package build system configuration.		04/09/2020 10:15 PM	2021-infrastructure-stable
3154	GROMACS	Task	Resolved	Low	Update use of Python subprocess for >=3.5		04/09/2020 10:15 PM	
2792	GROMACS	Task	New	High	Improvement of PME gather and spread CUDA kernels		03/18/2020 03:57 PM	
2522	GROMACS	Task	Resolved	Normal	OpenCL context duplication		03/11/2020 04:15 PM	future
3370	GROMACS	Task	New	High	Further improvements to GPU Buffer Ops and Comms		03/04/2020 01:38 PM	
3357	GROMACS	Task	New	Normal	Make sure "colvars" interoperates stably and smoothly with gromacs		03/04/2020 11:25 AM	
1852	GROMACS	Task	New	Normal	Remove group scheme		03/03/2020 09:03 PM	future
3279	GROMACS	Task	New	Low	Provide more advice for building client software		03/02/2020 11:54 AM	
3252	GROMACS	Task	New	Normal	Remove support for 32 bit architectures		03/01/2020 02:05 PM	
3365	GROMACS	Task	New	Low	consider making GPU bonded work independent from nonbonded		03/01/2020 01:11 PM	
3366	GROMACS	Task	New	Normal	Enforce compability of MdModules		02/28/2020 11:20 AM	
3220	GROMACS	Task	New	Normal	change rolling pruning scheduling with GPU update		02/25/2020 03:41 PM	2021-infrastructure-stable

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
3047	GROMACS	Task	Feedback wanted	Normal	Set required versions for GROMACS 2021		02/20/2020 11:42 AM	
3382	GROMACS	Task	Accepted	Normal	Split up t_inputrec		02/17/2020 05:28 PM	
2965	GROMACS	Task	In Progress	Normal	Performance of GPU direct communications		02/14/2020 12:38 PM	2021
3093	GROMACS	Task	In Progress	High	rework GPU direct halo-exchange related force reduction complexities		02/14/2020 11:35 AM	2021-infrastructure-stable
2675	GROMACS	Task	In Progress	Normal	bonded CUDA offload task		02/12/2020 05:54 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
3356	GROMACS	Task	New	Normal	Expose setting of random seed to API		01/29/2020 06:16 PM	2021
3325	GROMACS	Task	New	Normal	Allow complete re-initialization of a simulation		01/29/2020 05:13 PM	2021-refactoring
2698	GROMACS	Task	In Progress	Normal	gmxapi documentation integration		01/29/2020 03:59 PM	2021-infrastructure-stable
3360	GROMACS	Task	New	Normal	investigate the future of DD dynamic load balancing with GPU offload		01/29/2020 11:23 AM	
3287	GROMACS	Task	New	Normal	Deprecate make_ndx, use select instead		01/23/2020 01:16 PM	
3353	GROMACS	Task	New	Normal	Document gmx densmap output		01/23/2020 12:52 PM	
3308	GROMACS	Task	New	Normal	GPU update-constraints: Cycle counting for GPU launches		01/23/2020 11:54 AM	2021-infrastructure-stable
3330	GROMACS	Task	New	Normal	Compile list of codepaths for testing task assignment		01/22/2020 10:03 AM	2021-refactoring
3324	GROMACS	Task	New	Normal	Rework CMake handling of GPU code		01/22/2020 09:52 AM	2021-refactoring
3329	GROMACS	Task	New	Normal	Extend energy comparison testing framework		01/22/2020 09:51 AM	2021-refactoring
3327	GROMACS	Task	New	Normal	Refactor workload flags		01/22/2020 09:45 AM	2021-refactoring
3326	GROMACS	Task	New	Normal	Allow changing task assignment		01/22/2020 09:44 AM	2021-refactoring
2756	GROMACS	Task	In Progress	Normal	gmxapi integration testing		01/16/2020 05:12 PM	2021-refactoring
2839	GROMACS	Task	New	Normal	make module and file naming consistent		01/16/2020 05:11 PM	2021
2770	GROMACS	Task	New	Normal	change branch maintenance policy		01/16/2020 05:09 PM	2021
3033	GROMACS	Task	In Progress	Normal	Clean up and modernize googletest bundling and usage		01/16/2020 04:50 PM	2021-refactoring
3229	GROMACS	Task	New	Normal	Move checkpointing to the beginning of the MD step		01/16/2020 04:31 PM	2021-infrastructure-stable
3300	GROMACS	Task	New	Normal	Abandon docs/OpenCLTODOList.txt?		01/15/2020 02:46 PM	
2855	GROMACS	Task	New	Normal	Allow compiling GROMACS without C compiler		01/10/2020 12:06 PM	
3014	GROMACS	Task	In Progress	Normal	gmxapi example Python scripts		01/03/2020 11:00 AM	2021-infrastructure-stable
1925	GROMACS	Task	In Progress	Normal	remove concept of unilateral global communication		12/29/2019 10:35 AM	2021
2169	GROMACS	Task	New	Normal	remove 'continuation' mdp option		12/29/2019 10:31 AM	2021
2771	GROMACS	Task	New	Normal	Size independent Hessian for normal mode analysis		12/28/2019 10:50 AM	future
2059	GROMACS	Task	In Progress	Normal	Separate different types of data in t_state		12/27/2019 04:42 PM	2021

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
2697	GROMACS	Task	New	Normal	improve FFT library flavor/version reporting		12/27/2019 04:40 PM	future
2695	GROMACS	Task	New	Low	bonded GPU module timing		12/27/2019 04:40 PM	2021
2686	GROMACS	Task	New	Normal	add tests for gpu bonded interactions		12/27/2019 04:40 PM	2021
2976	GROMACS	Task	New	Normal	Basic math for Multidimensional arrays		12/27/2019 04:37 PM	2021
2988	GROMACS	Task	In Progress	Low	clean up and refactor code to modern standards		12/27/2019 04:37 PM	future
2992	GROMACS	Task	New	Normal	Split hw_opt in const user options and dynamic settings		12/27/2019 04:31 PM	future
2997	GROMACS	Task	New	Normal	improve performance of alchemical free energy calculations		12/27/2019 04:31 PM	2021
3001	GROMACS	Task	New	Normal	explore simplifying virial and shift force reduction		12/27/2019 04:30 PM	2021
3008	GROMACS	Task	New	Normal	verify block size choice of CUDA bonded kernel		12/27/2019 04:30 PM	2021
3031	GROMACS	Task	New	Normal	evaluate the impact of particle order on PME		12/27/2019 04:29 PM	2021
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
3268	GROMACS	Task	New	Normal	add more Intel driver recommendations		12/26/2019 04:39 PM	
3267	GROMACS	Task	New	Normal	Document tools		12/26/2019 03:20 PM	future
3262	GROMACS	Task	New	High	Trjconv - dimer protein-ligand		12/20/2019 09:26 PM	
3224	GROMACS	Task	New	Normal	add regression test case large enough to miscalculated GPU grid launch cases		12/20/2019 01:18 PM	2021
2671	GROMACS	Task	New	Normal	replace constants like M_PI		12/20/2019 01:17 PM	future
2773	GROMACS	Task	New	Normal	improve GPU error handling and make such handling uniform across modules		12/20/2019 01:09 PM	2021
2053	GROMACS	Task	New	Normal	refine notation in GPU code		12/20/2019 01:04 PM	2021
2524	GROMACS	Task	New	Normal	struct alignment/packing for OpenCL host & device code		12/20/2019 12:20 PM	future
2518	GROMACS	Task	New	Normal	redesign task-assignment code for OpenCL		12/20/2019 12:19 PM	future
2498	GROMACS	Task	New	Normal	OpenCL memory pinning/mapping		12/20/2019 12:18 PM	future
2475	GROMACS	Task	New	Normal	make OpenCL 1st class-citizen in the build system		12/20/2019 12:14 PM	2021
2353	GROMACS	Task	New	Normal	improve on relative tolerance for constructing tables		12/20/2019 12:12 PM	2021
1587	GROMACS	Task	New	Normal	improve the configurability of regression tests		12/20/2019 12:02 PM	2021
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
3010	GROMACS	Task	In Progress	Normal	upgrade OpenCL stack on bs-gpu01		12/20/2019 08:25 AM	2021-infrastructure-stable

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
3255	GROMACS	Task	New	Normal	Move benchmarking options from mdrun to a dedicated tool		12/19/2019 01:21 PM	
3254	GROMACS	Task	New	Normal	Remove support for generation of virtual sites to replace aromatic rings in standard residues		12/19/2019 12:13 PM	
3256	GROMACS	Task	New	Normal	Remove -nsteps option from mdrun		12/19/2019 12:12 PM	
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
2795	GROMACS	Task	New	Normal	Incorporate regressiontests into core gromacs		12/02/2019 01:44 PM	2021-infrastructure-stable
2481	GROMACS	Task	New	Low	Update gmx report-methods to write more method information		12/02/2019 01:22 PM	2021-infrastructure-stable
3212	GROMACS	Task	New	Normal	Update regression tests for new kernel flavours		11/21/2019 11:50 AM	
3201	GROMACS	Task	In Progress	Normal	Convert mdp parameters to key value tree		11/06/2019 06:06 PM	
3194	GROMACS	Task	New	Normal	consider passing GPU dependency list to both dependency producers and consumers		11/01/2019 07:10 PM	
3077	GROMACS	Task	Feedback wanted	Normal	PME/PP GPU Comms unique pointer deletion causes seg fault when CUDA calls exist in destructor		11/01/2019 06:56 PM	
3132	GROMACS	Task	New	Normal	gmxapi testing support tools		10/31/2019 03:35 PM	
3187	GROMACS	Task	New	Normal	Template updated PME kernels using threads per atom		10/30/2019 11:33 AM	
3186	GROMACS	Task	In Progress	Normal	Update Constant/Variable naming in the PME GPU kernels.		10/30/2019 11:23 AM	
3185	GROMACS	Task	New	Normal	Update PME CUDA kernels to allow a different number of threads per atom in the gather and spread kernels.		10/30/2019 11:18 AM	
3181	GROMACS	Task	New	Normal	consolidate task assignment and workload data initialization		10/28/2019 02:53 PM	
3153	GROMACS	Task	New	Low	Let CMake process module directories earlier to support more modern CMake idioms.		10/17/2019 10:40 AM	2021-infrastructure-stable
3123	GROMACS	Task	New	Normal	address sanitizer coverage of parallelization code-paths		10/05/2019 12:32 AM	
2947	GROMACS	Task	Accepted	Normal	make an end to end test for membed		09/24/2019 03:22 PM	future
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
3013	GROMACS	Task	New	Normal	Extend logging levels in MDLogger		09/06/2019 02:34 PM	2021-infrastructure-stable
3015	GROMACS	Task	New	Normal	Create central log handle for calls to gmx_fatal		09/06/2019 02:34 PM	2021-infrastructure-stable
3078	GROMACS	Task	New	Normal	Allow MD modules to register energy output fields themselves		09/06/2019 11:36 AM	
988	GROMACS	Task	New	Normal	Definition of "public API"		08/28/2019 02:50 PM	future
2905	GROMACS	Task	New	Normal	Add a Jenkins configuration with std library assert		08/24/2019 05:22 PM	
2341	GROMACS	Task	New	Low	assess the state of building and using GROMACS on Windows		07/29/2019 11:09 PM	future
3016	GROMACS	Task	New	Normal	intermittent failure of essentialdynamics test		07/18/2019 05:23 PM	
3040	GROMACS	Task	New	Normal	Refactor Restraint module		07/18/2019 03:59 PM	
2983	GROMACS	Task	New	Normal	better suited data-types for bonded GPU kernels		07/11/2019 04:32 PM	
3005	GROMACS	Task	New	Normal	Move logging in gmx preprocess to MDLogger		06/26/2019 10:01 AM	

#	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	
3003	GROMACS	Task	New	Normal	implement heuristic fallback to CPU when there is too little work for GPU offload		06/25/2019 04:10 PM	
3002	GROMACS	Task	New	Normal	consider splitting bonded work into local/nonlocal		06/25/2019 04:06 PM	
2375	GROMACS	Task	New	Normal	Clarify execution phases for MD simulation		04/30/2019 12:59 PM	
2933	GROMACS	Task	New	Normal	Convert walls to a ForceProvider		04/25/2019 02:43 PM	
2919	GROMACS	Task	New	Normal	C++ style guidelines for namespace use		04/15/2019 01:21 PM	
2909	GROMACS	Task	New	Normal	consider implementing mechanisms to ensure pair lists are not used past their max lifetime		04/03/2019 05:14 PM	
2898	GROMACS	Task	New	Low	Naming common variables		03/26/2019 11:46 PM	
2863	GROMACS	Task	New	Normal	improve PBC handling		03/11/2019 04:28 PM	
701	GROMACS	Task	New	Normal	Add symbol visibility macros		03/02/2019 01:46 AM	future
2519	GROMACS	Task	New	High	Improve/remove PME OpenCL kernel barriers		02/15/2019 06:34 PM	
1862	GROMACS	Task	New	Normal	Fully replace t_topology by gmx_mtop_t		02/13/2019 04:53 PM	
2835	GROMACS	Task	New	Normal	Matrix class constraint to upper or lower triangle		02/07/2019 02:44 PM	
2857	GROMACS	Task	New	Normal	Clarify recommended function specifies (constexpr, noexcept, pure)		02/04/2019 04:48 AM	
2851	Support Platforms	Task	New	Normal	uninstall redmine checklist plugin		01/30/2019 03:33 PM	
2796	GROMACS	Task	New	Low	clarify what mdrun -cpt means		01/03/2019 02:09 PM	
2672	GROMACS	Task	New	Normal	check & document execution width requirements in OpenCL		12/31/2018 11:20 AM	future
2650	GROMACS	Task	New	Normal	revise OpenCL stack recommendations		12/31/2018 11:19 AM	future
2528	GROMACS	Task	New	Normal	PME GPU tuning		12/31/2018 11:18 AM	future
2674	GROMACS	Task	Accepted	Normal	Improve domain decomposition for bilayer systems		12/07/2018 04:03 PM	future
2787	GROMACS	Task	New	Normal	allow passing flags to allocateDeviceBuffer		12/03/2018 01:54 PM	
2632	GROMACS	Task	New	Low	make sure cmake defines proper hwloc versionc with cross-compilation enabled		12/03/2018 01:35 PM	future
1879	GROMACS	Task	In Progress	Low	make the GROMACS OpenCL kernel work on Gallium		11/30/2018 05:46 PM	future
2758	GROMACS	Task	New	Low	Modernize genconf		11/15/2018 07:38 AM	future
2527	GROMACS	Task	New	Normal	Rename GpuEventSynchronizer to something more fitting (after mergin PME OpenCL)		10/30/2018 04:06 AM	future
2521	GROMACS	Task	New	Normal	Implement alternating PME/NB wait for OpenCL		10/15/2018 12:39 PM	
2682	GROMACS	Task	New	Normal	Add MSAN configuration		10/09/2018 06:28 PM	
2670	GROMACS	Task	New	Low	remove old/backward compatibility OpenCL support from releng		10/04/2018 06:06 PM	
2304	GROMACS	Task	New	Normal	Document and propose tracking mdrun heuristics		10/03/2018 09:39 PM	future

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
2115	GROMACS	Task	New	Normal	trjconv does too many things, and combinations of them work poorly		10/02/2018 09:04 AM	
2367	GROMACS	Task	New	Normal	construct pbc_simd less often		09/24/2018 11:02 PM	future
2608	GROMACS	Task	New	Normal	Remove code duplication between OpenCL and CUDA		09/24/2018 12:47 PM	
2530	GROMACS	Task	New	Normal	consider using CUDA Driver API		09/23/2018 11:47 PM	future
2616	GROMACS	Task	New	Normal	Model for MD state		09/14/2018 05:12 PM	
2531	GROMACS	Task	New	Low	Consider optimizing tabulated data access on GPU		07/30/2018 12:31 PM	
2010	GROMACS	Task	New	Normal	Use size_t instead of int for indexing		07/01/2018 07:57 AM	
2535	GROMACS	Task	New	Normal	consider compiling opencl fft kernels once		05/31/2018 01:33 PM	
2514	GROMACS	Task	New	Normal	PME OpenCL reductions with intrinsics		05/31/2018 12:27 AM	future
2532	GROMACS	Task	New	Normal	enable queue priorities in OpenCL		05/29/2018 02:29 PM	
2520	GROMACS	Task	New	Normal	Treat OpenCL kernel width more diligently		05/24/2018 06:21 PM	
2496	GROMACS	Task	New	Low	find system xdr properly		05/02/2018 02:19 PM	
2488	GROMACS	Task	New	Normal	use MPI non-blocking collectives to overlap pull comm		04/25/2018 04:19 PM	
2478	GROMACS	Task	New	Low	avoid use of getenv in static initialization		04/13/2018 11:57 AM	
2469	GROMACS	Task	New	Normal	implement GPU timer reduction for reporting		03/27/2018 05:08 PM	
2464	GROMACS	Task	New	Normal	GPU performance goals overview		03/26/2018 10:42 AM	
2463	GROMACS	Task	New	Low	PME GPU decomposition		03/26/2018 10:42 AM	
2402	GROMACS	Task	New	Normal	PME kernels general performance improvements		03/26/2018 10:41 AM	future
2462	GROMACS	Task	New	Normal	consider adding STL misuse tests		03/23/2018 01:23 AM	
2448	GROMACS	Task	Accepted	Normal	should mdrun -multidir permit only one directory?		03/21/2018 12:10 PM	
2412	GROMACS	Task	New	Normal	attempt to do better FFTW planning		03/15/2018 05:01 PM	
2456	GROMACS	Task	New	Normal	Add a pull module external potential tests		03/15/2018 03:02 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	
2435	GROMACS	Task	New	Normal	identify and note about/tune task offload in GPU-bound runs		03/02/2018 04:08 PM	
2422	GROMACS	Task	New	Normal	write C kernel for tables in Verlet scheme		02/26/2018 01:38 PM	
2221	GROMACS	Task	New	Normal	Avoid preprocessor for SIMD functions		02/21/2018 01:43 PM	
2376	GROMACS	Task	New	Normal	max_mpi_ranks has wrong name		02/10/2018 11:03 AM	
1971	GROMACS	Task	New	Normal	Removing buggy features vs. keeping workflows		01/19/2018 01:36 PM	future
2382	GROMACS	Task	New	Normal	Simplify Doxygen guidelines		01/13/2018 12:40 AM	
2175	GROMACS	Task	New	Normal	improve clang static analyzer docs further		01/04/2018 04:13 PM	future
2371	GROMACS	Task	New	Normal	mtop searching needs reconsideration		01/04/2018 11:54 AM	future
2092	GROMACS	Task	New	Normal	Tests running on GPU, and hardware assignment		12/19/2017 05:27 PM	future

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
2351	GROMACS	Task	New	Normal	Avoid the SIMD module depending on non-trivial parts of Gromacs		12/14/2017 02:47 AM	future
2294	GROMACS	Task	New	Normal	Require identical hardware on nodes on parallel runs		11/19/2017 08:54 PM	
2240	GROMACS	Task	Accepted	Low	GPU emulation mode support for PME missing		09/16/2017 10:02 PM	
1309	Support Platforms	Task	New	Normal	Jenkins verification improvements		06/01/2017 02:34 PM	
2185	GROMACS	Task	New	Normal	add docs on MPI + CUDA w/wo MPS		05/24/2017 05:17 PM	
2182	GROMACS	Task	New	Low	de-duplicate code in densorder and hydorder		05/16/2017 11:29 AM	
2178	GROMACS	Task	New	Normal	Move checks for specific warnings to source repo		05/12/2017 03:57 PM	
2168	GROMACS	Task	Feedback wanted	Normal	Design for multiple comparisons against same test reference data		05/08/2017 02:45 PM	future
2166	GROMACS	Task	Accepted	Normal	gmx trjconv functionality should check for mismatch between the tpr and the trajectory		05/05/2017 04:32 PM	
652	GROMACS	Task	Blocked, need info	Normal	Change selection method implementation to use C++		04/23/2017 08:05 PM	future
2158	GROMACS	Task	New	Normal	consider adding post-submit test that runs PME with 2xNN kernels		04/19/2017 08:04 PM	
2035	GROMACS	Task	New	Normal	A common trajectory analysis data exchange format		03/15/2017 05:46 PM	future
2133	GROMACS	Task	New	Low	gmx traj needs reform		03/07/2017 02:02 PM	
2055	GROMACS	Task	New	Low	Wiki registration is broken		01/20/2017 11:31 AM	
2089	GROMACS	Task	New	Normal	Encourage code review		01/10/2017 12:03 AM	
2084	GROMACS	Task	New	Low	MPI and stderr/log output		11/28/2016 06:37 PM	
1829	GROMACS	Task	New	Normal	Future of thread level parallelism		11/18/2016 05:29 PM	
1170	GROMACS	Task	New	Normal	mdlib reorganization		11/17/2016 03:47 PM	future
2069	GROMACS	Task	New	Low	Simple thread-parallelism inside routines		11/09/2016 06:06 PM	
1768	GROMACS	Task	New	Normal	decide future of command-line options vs env vars		11/03/2016 05:51 PM	future
1815	Support Platforms	Task	In Progress	Normal	implement and execute plan for new releng machinery		10/15/2016 05:37 PM	
2048	GROMACS	Task	New	Normal	C++11: CUDA dependency on general headers		09/07/2016 10:30 PM	
1907	GROMACS	Task	Accepted	Low	keeping compile- and run-time CPU/arch detection consistent		08/01/2016 10:09 PM	
2009	GROMACS	Task	New	Normal	improve command-line reporting of useful things		07/26/2016 12:54 PM	
838	GROMACS	Task	New	Normal	Improve generic error reporting routines		07/11/2016 08:29 PM	
1017	GROMACS	Task	New	Normal	C++ Vector/Matrix classes		07/11/2016 08:23 PM	
1140	GROMACS	Task	New	Normal	Class design for passing options and data		07/11/2016 08:19 PM	

...