

Issues

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
3134	GROMACS	Feature	Feedback wanted	Normal	gmxapi Python exception names may need improvement	Eric Irrgang	10/13/2019 01:50 PM	
3058	GROMACS	Bug	Feedback wanted	Normal	Error when using a large PME grid on a GPU		09/04/2019 07:26 PM	
3055	GROMACS	Bug	Feedback wanted	Normal	Error in gmx xpm2ps		08/22/2019 03:27 PM	
3028	GROMACS	Bug	Feedback wanted	Normal	install fail on Centos 6		07/15/2019 12:32 PM	
2927	GROMACS	Bug	Feedback wanted	Low	CMake 3.14.1 fails to properly run gmxDetectCpu.make		10/01/2019 11:13 AM	2019.5
2828	GROMACS	Bug	Feedback wanted	Normal	Installation issue on Power 9 system with SIMD support		01/18/2019 11:54 AM	
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	
2513	GROMACS	Bug	Feedback wanted	Normal	ref_t and temperature incorrect with coulomb-type = user	Yu Du	05/31/2018 04:05 PM	
2482	GROMACS	Bug	Feedback wanted	Normal	Atoms/molecules in freezegrps move and system crashes		05/18/2018 07:13 PM	
2390	GROMACS	Bug	Feedback wanted	Normal	GROMACS build system should check for valid nvcc flags before use		01/30/2019 06:16 PM	2020
2218	GROMACS	Feature	Feedback wanted	Normal	A tiny feature: damping for umbrella pull		08/16/2017 07:20 PM	
2168	GROMACS	Task	Feedback wanted	Normal	Design for multiple comparisons against same test reference data		05/08/2017 02:45 PM	future
2147	GROMACS	Bug	Feedback wanted	Normal	Parrinello-Rahman barostat not properly working		06/06/2017 07:53 AM	
1977	GROMACS	Bug	Feedback wanted	Low	warning: __WORDSIZE not defined		09/21/2018 06:19 PM	2020
1880	GROMACS	Bug	Feedback wanted	Normal	PP-PME load balancing issue	Berk Hess	10/03/2018 09:45 PM	future
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	
1442	GROMACS	Bug	Feedback wanted	Normal	Not consistent solvation free energies differences	Michael Shirts	07/11/2016 08:13 PM	
1377	GROMACS	Feature	Feedback wanted	Low	Replica exchange if replicas not in ascendent T	David van der Spoel	06/23/2016 03:48 PM	
1551	Support Platforms	Bug	Feedback wanted	Normal	git index.lock issue		05/31/2017 05:37 PM	

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694	Support Platforms	Feature	Feedback wanted	Normal	Write instructions/policy for issue handling	Rossen Apostolov	05/31/2017 05:41 PM	
1252	TNG trajectory library	Bug	Feedback wanted	Normal	residual ids and atomIDs	Magnus Lundborg	06/12/2013 10:35 AM	version 1
3144	GROMACS	Bug	Resolved	Normal	gmxapi.mdrun does not clearly expose the output trajectory.	Eric Irrgang	10/21/2019 09:30 AM	2020-beta2
3120	GROMACS	Bug	Resolved	High	Uninitialized energy and virial contributions with PME on GPU on PME-only rank		10/09/2019 11:15 AM	2019.5
3118	GROMACS	Task	Resolved	Normal	clang-tidy segfaulting in CI		10/18/2019 07:31 PM	2020-beta2
3061	GROMACS	Task	Resolved	Normal	support for Zen2		10/21/2019 07:11 PM	2020-beta2
2912	GROMACS	Task	Resolved	Normal	C++ extension module for Python bindings	Eric Irrgang	07/05/2019 09:00 AM	
2895	GROMACS	Task	Resolved	Normal	gmxapi Output proxy establishes execution dependency.	Eric Irrgang	03/29/2019 05:18 PM	2020
2894	GROMACS	Task	Resolved	Normal	Wrap importable Python code.	Eric Irrgang	05/09/2019 11:30 AM	2020
2893	GROMACS	Task	Resolved	Normal	Integrate gmxapi Python package	Eric Irrgang	04/09/2019 12:20 PM	2020
2623	GROMACS	Task	Resolved	Normal	Allow extensible MDModules and forceProviders.		10/15/2018 03:44 PM	
2586	GROMACS	Feature	Resolved	Normal	Versioned libgmxapi target for build, install, headers, docs		03/02/2019 01:32 AM	
2585	GROMACS	Feature	Resolved	Normal	Infrastructure supporting external API		03/31/2019 04:47 PM	
2453	GROMACS	Task	Resolved	High	PME OpenCL porting effort	Aleksei lupinov	06/05/2019 05:32 PM	2020
2451	GROMACS	Feature	Resolved	Normal	Linear virtual sites with fixed distance	David van der Spoel	09/16/2019 01:15 PM	
1967	Support Platforms	Bug	Resolved	Normal	Documentation pages generated by Jenkins do not render properly		08/27/2016 02:04 AM	
837	Support Platforms	Task	Resolved	Low	Consider subproject organization of the Gromacs project		07/14/2014 12:07 PM	
2188	TNG trajectory library	Feature	Resolved	High	Masses missing from TNG specification	Magnus Lundborg	06/13/2017 05:08 PM	
1229	TNG trajectory library	Feature	Resolved	Normal	Selection groups	Magnus Lundborg	11/29/2013 04:38 PM	version 1
3101	GROMACS	Bug	Blocked, need info	Normal	detect compilation failed		09/24/2019 05:26 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	
2733	GROMACS	Bug	Blocked, need info	Normal	MdrunUtilityMpiUnitTests timesout on i686 and armv7hl with OpenMPI 2.1.5	Paul Bauer	11/08/2018 04:27 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	
921	GROMACS	Feature	Blocked, need info	Normal	Default index groups and selections		07/11/2016 08:27 PM	

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652	GROMACS	Task	Blocked, need info	Normal	Change selection method implementation to use C++		04/23/2017 08:05 PM	future
3111	GROMACS	Bug	Fix uploaded	Low	sample_restraint testing should not download files	Eric Irrgang	10/16/2019 06:00 PM	2020-beta2
3085	GROMACS	Bug	Fix uploaded	High	gromacs-toolchain.cmake file does not work on OS X		10/06/2019 04:59 PM	2020-beta2
2859	GROMACS	Task	Fix uploaded	Normal	Change ArrayRef iterator type from pointer to std::iterator		02/08/2019 11:00 PM	
2628	GROMACS	Bug	Fix uploaded	Normal	GMXRC removes trailing colon from existing MANPATH		08/28/2018 03:13 PM	
1985	GROMACS	Bug	Fix uploaded	Low	CUDA build system refactoring awaiting review		10/15/2018 05:21 PM	2020
1030	GROMACS	Feature	Fix uploaded	Low	adding -tu option to some analysis tools	Rossen Apostolov	07/11/2016 08:22 PM	
2180	Support Platforms	Feature	Fix uploaded	Low	releng matrices would work better with a hint for execution		05/19/2017 01:02 AM	
3151	GROMACS	Bug	In Progress	Normal	integrator md-vv does not print at nstlog	Pascal Merz	10/17/2019 02:23 AM	2020-beta2
3100	GROMACS	Bug	In Progress	Normal	crash with GPU comm DD		09/27/2019 01:28 PM	2020-beta2
3033	GROMACS	Task	In Progress	Normal	Clean up and modernize googletest bundling and usage		08/24/2019 05:23 PM	2021-infrastructure-stable
3029	GROMACS	Feature	In Progress	High	GPU force buffer ops + reduction		10/11/2019 11:55 AM	2020-beta2
3027	GROMACS	Task	In Progress	Normal	Move sample_restraint development from GitHub to Gerrit	Eric Irrgang	09/24/2019 03:23 PM	2020-beta2
3010	GROMACS	Task	In Progress	Normal	upgrade OpenCL stack on bs-gpu01		08/23/2019 03:23 PM	2020-infrastructure-update-post-beta1
2998	GROMACS	Task	In Progress	Normal	Update Python detection		08/16/2019 09:57 AM	2020-infrastructure-update-post-beta1
2988	GROMACS	Task	In Progress	Low	clean up and refactor code to modern standards		06/20/2019 02:14 PM	2020
2899	GROMACS	Task	In Progress	Normal	Update testing matrix versions for GROMACS 2020 release	Mark Abraham	10/12/2019 09:44 PM	2020-infrastructure-update-post-beta1
2896	GROMACS	Feature	In Progress	Normal	Python packaging		10/09/2019 04:08 PM	2020
2862	GROMACS	Bug	In Progress	Normal	Division by zero in restrained dihedrals		04/01/2019 11:53 AM	2020
2850	GROMACS	Task	In Progress	Normal	assess Raptor Talos for testing	Szilárd Páll	02/12/2019 01:14 PM	
2818	GROMACS	Task	In Progress	Normal	bonded GPU kernel fusion	Magnus Lundborg	07/03/2019 09:01 PM	
2817	GROMACS	Feature	In Progress	High	GPU X/F buffer ops		10/11/2019 11:55 AM	2020-beta2
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
2766	GROMACS	Task	In Progress	Normal	Improve hardware option selection	Kevin Boyd	12/20/2018 06:40 PM	2020
2756	GROMACS	Task	In Progress	Normal	gmxapi integration testing		08/16/2019 09:56 AM	2020-infrastructure-update-post-beta1
2734	GROMACS	Bug	In Progress	Normal	regressiontests/kernel core dumps on ppc64le	Paul Bauer	06/15/2019 04:12 PM	future
2727	GROMACS	Task	In Progress	Low	Move non-analysis functions out of gmxana		01/20/2019 07:48 PM	2020
2696	GROMACS	Task	In Progress	Normal	ensure PME queue is flushed	Szilárd Páll	12/31/2018 11:21 AM	future
2675	GROMACS	Task	In Progress	Normal	bonded CUDA offload task		06/26/2019 08:38 PM	2020
2620	GROMACS	Feature	In Progress	Normal	MD signaling API		03/02/2019 01:24 AM	

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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	
2452	GROMACS	Task	In Progress	Normal	Reduce data dependencies in mdrun algorithms	Berk Hess	03/14/2018 08:47 PM	
2426	GROMACS	Feature	In Progress	Normal	Trajectory analysis tool for functional mode analysis by partial least squares fitting (PLS-FMA)		10/03/2018 11:31 PM	future
2395	GROMACS	Task	In Progress	Normal	break up commrec	Mark Abraham	09/19/2018 03:13 PM	2020
2368	GROMACS	Task	In Progress	Normal	update implementation of gmx msd	Kevin Boyd	11/03/2018 07:43 PM	future
2281	GROMACS	Task	In Progress	Normal	Represent data on regularly spaced N-dimensional grids.	Christian Blau	08/06/2019 08:48 AM	2020
2238	GROMACS	Task	In Progress	Normal	GPU emulation mode support for rolling pruning missing	Berk Hess	12/21/2017 03:21 PM	
2111	GROMACS	Feature	In Progress	Normal	Implement Gaussian screening of electrostatics		02/23/2019 12:33 PM	
2071	GROMACS	Task	In Progress	High	Low accuracy default settings yield incorrect liquid densities	Berk Hess	01/05/2018 03:32 PM	
2070	GROMACS	Feature	In Progress	Normal	Physical validation testing	Michael Shirts	10/12/2018 10:36 PM	2020
2059	GROMACS	Task	In Progress	Normal	Separate different types of data in t_state		10/12/2018 10:36 PM	2020
2017	GROMACS	Task	In Progress	Normal	Modularize simulation option storage and reading from mdp files	Christian Blau	04/06/2018 06:07 PM	future
1925	GROMACS	Task	In Progress	Normal	remove concept of unilateral global communication		07/15/2019 06:42 PM	2020
1879	GROMACS	Task	In Progress	Low	make the GROMACS OpenCL kernel work on Gallium		11/30/2018 05:46 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	
1627	GROMACS	Feature	In Progress	Normal	DPD integrator		07/11/2016 08:08 PM	
1618	GROMACS	Bug	In Progress	Normal	g_protonate segfaults unconditionally	Erik Lindahl	08/17/2015 02:10 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	
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
1083	GROMACS	Feature	In Progress	Normal	Improve collective error/warning/note handling in mdrun		07/11/2016 08:21 PM	
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
1010	GROMACS	Task	In Progress	Normal	Better support for multiple AnalysisData datasets	Teemu Murtola	07/11/2016 08:23 PM	
920	GROMACS	Task	In Progress	Normal	Add test framework for trajectory analysis modules	Teemu Murtola	07/11/2016 08:27 PM	
895	GROMACS	Feature	In Progress	Normal	g_rmsf previous frame as reference		04/29/2013 07:39 PM	future
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	
868	GROMACS	Feature	In Progress	Normal	Implement parallelization support to analysis framework	Kevin Boyd	02/07/2019 02:08 AM	2020

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867	GROMACS	Task	In Progress	Normal	Update Doxygen documentation for C++ code	Teemu Murtola	07/11/2016 08:28 PM	
438	GROMACS	Feature	In Progress	Low	New tool: g_correl	Alexey Shvetsov	06/20/2014 10:38 AM	future
1815	Support Platforms	Task	In Progress	Normal	implement and execute plan for new releng machinery		10/15/2016 05:37 PM	
1731	Support Platforms	Bug	In Progress	Normal	document jenkins configuration and set up means to track changes		05/31/2017 06:13 PM	
629	Support Platforms	Task	In Progress	Normal	List of users needs cleanup	Rossen Apostolov	02/21/2018 02:07 PM	
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
3155	GROMACS	Task	Accepted	Normal	Unify DD and CPU-GPU gather & scatter	Artem Zhmurov	10/17/2019 03:50 PM	2021-infrastructure-stable
3071	GROMACS	Bug	Accepted	Normal	complex.nbnxn-ljpme-LB-geometric failing with OpenCL timing debug mode assertions	Szilárd Páll	09/02/2019 10:19 PM	2020
2979	GROMACS	Task	Accepted	Normal	Reconsider default 1 OpenMP thread per thread-MPI rank	Berk Hess	09/24/2019 03:22 PM	2020-beta2
2947	GROMACS	Task	Accepted	Normal	make an end to end test for membed		09/24/2019 03:22 PM	future
2875	GROMACS	Task	Accepted	Normal	SIMD version of the free-energy kernel	Berk Hess	08/26/2019 03:47 PM	2020
2822	GROMACS	Task	Accepted	Normal	Make nbnxn a module	Berk Hess	01/03/2019 03:07 PM	2020
2737	GROMACS	Bug	Accepted	Low	AMD OpenCL fails release build in complex tests	Szilárd Páll	10/14/2019 09:16 PM	2020-beta2
2706	GROMACS	Task	Accepted	Normal	Rework classic QM/MM interface		11/05/2018 10:06 AM	2020
2702	GROMACS	Bug	Accepted	Normal	PME gather reduction race in OpenCL (and CUDA)		03/28/2019 03:14 PM	
2674	GROMACS	Task	Accepted	Normal	Improve domain decomposition for bilayer systems		12/07/2018 04:03 PM	future
2615	GROMACS	Feature	Accepted	Normal	Switch to Python3		07/05/2019 02:57 PM	2020
2581	GROMACS	Feature	Accepted	Normal	User interface for hybrid Monte Carlo		10/15/2018 05:21 PM	2020
2553	GROMACS	Bug	Accepted	Normal	Incorrect COM velocity correction with frozen atoms	Berk Hess	12/03/2018 01:15 PM	2020
2448	GROMACS	Task	Accepted	Normal	should mdrun -multidir permit only one directory?		03/21/2018 12:10 PM	
2391	GROMACS	Task	Accepted	Normal	re-enable TPI test	Berk Hess	01/09/2019 05:17 PM	2020
2310	GROMACS	Feature	Accepted	Low	Let mdrun dump coordinates with non-finite energy		10/03/2018 09:47 PM	future
2288	GROMACS	Feature	Accepted	Low	gmx msd doesn't optimally handle missing input trajectory frames		11/10/2017 11:03 AM	
2240	GROMACS	Task	Accepted	Low	GPU emulation mode support for PME missing		09/16/2017 10:02 PM	
2233	GROMACS	Bug	Accepted	Normal	replica exchange and -append bugged?		03/05/2018 01:38 PM	

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2194	GROMACS	Feature	Accepted	Low	xvg output requested as an output option in place of xpm files		05/31/2017 04:26 PM	
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	12/03/2018 01:25 PM	2020
2166	GROMACS	Task	Accepted	Normal	gmx trjconv functionality should check for mismatch between the tpr and the trajectory		05/05/2017 04:32 PM	
2107	GROMACS	Task	Accepted	High	Change to clang-format		08/02/2019 07:30 PM	
2054	GROMACS	Feature	Accepted	High	PME on GPU	Aleksei lupinov	10/03/2019 09:41 PM	2020
1964	GROMACS	Feature	Accepted	Normal	"pull=no" should not produce warnings about "unknown" pull keywords		05/20/2016 02:37 PM	
1943	GROMACS	Task	Accepted	Low	make sure releases are submitted early for Debian Experimental	Szilárd Páll	12/31/2018 11:15 AM	2020
1919	GROMACS	Bug	Accepted	Normal	static linking issues cause by hwloc support		10/12/2018 10:49 PM	future
1907	GROMACS	Task	Accepted	Low	keeping compile- and run-time CPU/arch detection consistent		08/01/2016 10:09 PM	
1902	GROMACS	Feature	Accepted	Low	Add grompp check that non-excluded atoms are not too close to each other in the starting structure		02/15/2016 01:34 PM	
1839	GROMACS	Bug	Accepted	Low	pdb2gmx: Failure to rename non-standard hydrogen atom names after generating missing hydrogens in pdb2gmx		07/09/2016 07:27 PM	future
1781	GROMACS	Task	Accepted	Normal	re-design benchmarking functionality	Mark Abraham	10/08/2018 07:04 PM	2020
1511	GROMACS	Feature	Accepted	Normal	add PDBx (ie mmcif) support		10/05/2018 07:14 PM	
1328	GROMACS	Feature	Accepted	Normal	Names for selection positions		07/11/2016 08:15 PM	
1221	GROMACS	Feature	Accepted	Normal	More generic position mapping for selections		06/10/2014 02:58 PM	future
1192	GROMACS	Feature	Accepted	Normal	Add support for Verlet scheme with Buckingham	Berk Hess	07/11/2016 08:19 PM	
1165	GROMACS	Feature	Accepted	Low	Multi-SIMD binaries		01/23/2019 02:08 PM	2020
1056	GROMACS	Task	Accepted	Normal	status of fft5d_threads and fftw3_threads functionality	Mark Abraham	07/11/2016 08:21 PM	
907	GROMACS	Feature	Accepted	Normal	Add tests for verifying installed headers		03/11/2014 09:15 PM	future
720	GROMACS	Feature	Accepted	Low	permit pdb2gmx to choose a kind of HIS based on proton position		11/17/2016 03:51 PM	future
1106	Benchmark suite	Feature	New	Normal	publish benchmark numbers		06/19/2014 12:08 PM	
1105	Benchmark suite	Feature	New	Normal	produce a benchmark suite		09/13/2016 10:31 PM	
3172	GROMACS	Feature	New	Normal	QM/MM Interface with CP2K	Dmitry Morozov	10/22/2019 12:35 PM	future
3171	GROMACS	Task	New	Normal	schedule CPU H2D force contribution in separate stream		10/22/2019 12:19 AM	2020
3170	GROMACS	Task	New	Low	investigate GPU f buffer ops use cases		10/22/2019 12:14 AM	2020

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3168	GROMACS	Feature	New	Normal	GPU update release notes		10/21/2019 04:10 PM	
3167	GROMACS	Task	New	Normal	GPU update path user documentation		10/21/2019 04:09 PM	2020-beta3
3166	GROMACS	Bug	New	Normal	Compilation failing on Ubuntu 19.04 with Cuda 10.1		10/19/2019 09:13 PM	
3165	GROMACS	Bug	New	Normal	task assignment silent abort		10/18/2019 07:46 PM	
3164	GROMACS	Bug	New	Normal	mdrun-mpi-test with separate PME ranks and PP-PME CPU comm crashes		10/18/2019 07:34 PM	2020-beta2
3163	GROMACS	Bug	New	High	gpuupdate / task assignment stabilization	Artem Zhmurov	10/21/2019 03:59 PM	2020-beta2
3162	GROMACS	Feature	New	Normal	Add virtual site support to GPU version of update-constraints.		10/21/2019 03:59 PM	
3161	GROMACS	Bug	New	Normal	mdrun-test hangs with -ntmpi2		10/17/2019 05:34 PM	2020
3160	GROMACS	Feature	New	High	implement direct comm for different src/target memory spaces	Alan Gray	10/22/2019 06:11 PM	2020
3159	GROMACS	Task	New	High	eliminate regression due to moving gmx_pme_send_coordinates()	Alan Gray	10/17/2019 02:57 PM	2020
3158	GROMACS	Task	New	Normal	use MPI_Isend() in sendFTtoPpCudaDirect and receiveCoordinatesFromPpCudaDirect	Alan Gray	10/17/2019 02:48 PM	
3157	GROMACS	Task	New	Normal	separate PME x receive sync	Alan Gray	10/17/2019 02:44 PM	
3156	GROMACS	Task	New	Normal	move ddUsesGpuDirectCommunication and related conditionals into the workload data structures	Alan Gray	10/17/2019 02:00 PM	2020-beta3
3154	GROMACS	Task	New	Low	Update use of Python subprocess for >=3.5		10/17/2019 01:46 PM	
3153	GROMACS	Task	New	Low	Let CMake process module directories earlier to support more modern CMake idioms.		10/17/2019 10:40 AM	2021-infrastructure-stable
3152	GROMACS	Feature	New	Low	Infrastructure and patterns for expressing public interfaces		10/17/2019 10:40 AM	2021-infrastructure-stable
3150	GROMACS	Bug	New	Normal	gmxapi data type annotations are confusing and inadequate	Eric Irrgang	10/22/2019 03:08 PM	2021-infrastructure-stable
3149	GROMACS	Feature	New	Normal	Python user interface for obtaining simulation artifacts as files.	Eric Irrgang	10/15/2019 06:21 PM	
3148	GROMACS	Feature	New	Normal	Roadmap for gmxapi filesystem interactions.	Eric Irrgang	10/15/2019 06:23 PM	2021-infrastructure-stable
3147	GROMACS	Feature	New	Normal	gmxapi workflow checkpointing	Eric Irrgang	10/15/2019 06:18 PM	2021-infrastructure-stable
3143	GROMACS	Task	New	Normal	move the non-force accumulation/accounting tasks out of the GPU wait functions	Szilárd Páll	10/14/2019 05:14 PM	2020
3142	GROMACS	Feature	New	High	centralize and clarify GPU force buffer clearing		10/14/2019 04:56 PM	2020-beta2
3141	GROMACS	Bug	New	Normal	gmxapi File placeholders missing from beta release	Eric Irrgang	10/15/2019 03:57 PM	2020
3140	GROMACS	Feature	New	Normal	Allow explicit input definition for gmxapi.operation function wrapper	Eric Irrgang	10/15/2019 03:56 PM	2020
3139	GROMACS	Task	New	Normal	gmxapi Futures should be subscribable	Eric Irrgang	10/15/2019 03:56 PM	

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3138	GROMACS	Feature	New	Normal	Improve ensemble support in Context specification.		10/15/2019 03:56 PM	
3136	GROMACS	Bug	New	Normal	gmxapi.operation data flow topology unclear or incomplete	Eric Irrgang	10/22/2019 03:09 PM	2020-beta3
3135	GROMACS	Feature	New	Normal	Make GPU traits into opaque types		10/14/2019 10:24 AM	
3133	GROMACS	Task	New	Normal	Cookiecutter for sample_restraint	Eric Irrgang	10/13/2019 01:07 PM	2020
3132	GROMACS	Task	New	Low	gmxapi testing support tools		10/13/2019 01:00 PM	
3131	GROMACS	Task	New	Normal	support ccache with clang-tidy	Mark Abraham	10/15/2019 07:23 AM	
3130	GROMACS	Task	New	Normal	Interim handling of gmxapi data references.	Eric Irrgang	10/22/2019 03:09 PM	2020-beta3
3128	GROMACS	Task	New	High	do not fall back to CPU path on energy-only steps	Alan Gray	10/11/2019 11:55 AM	2020-beta2
3127	GROMACS	Bug	New	Normal	mddrun-mpi-test -ntmpi 2 runs out of memory with OpenCL on Nvidia		10/09/2019 05:33 PM	
3126	GROMACS	Feature	New	Normal	State propagator GPU data manager		10/09/2019 02:42 PM	
3125	GROMACS	Bug	New	Normal	OpenCL on Volta and Turing broken		10/13/2019 11:46 PM	2020-beta2
3124	GROMACS	Bug	New	Normal	significant performance loss due to DLB auto-off when PP/PME load >1		10/09/2019 04:33 PM	
3123	GROMACS	Task	New	Normal	address sanitizer coverage of parallelization code-paths		10/05/2019 12:32 AM	
3119	GROMACS	Task	New	Normal	clang-tidy coverage of parallelization codepaths		10/04/2019 12:17 PM	2020
3117	GROMACS	Feature	New	Normal	Coulomb FEP PME on GPU	Magnus Lundborg	10/04/2019 09:16 AM	future
3116	GROMACS	Bug	New	Normal	regressiontests/freeenergy core dumps on ppc64le	Paul Bauer	10/04/2019 10:52 PM	
3115	GROMACS	Feature	New	Normal	Device stream manager		10/04/2019 09:00 AM	
3114	GROMACS	Task	New	Low	Possible improvements to update-constraints	Artem Zhmurov	10/07/2019 11:38 AM	
3113	GROMACS	Bug	New	Low	Use of read_tps_conf is deprecated	Paul Bauer	10/01/2019 11:36 AM	2021-infrastructure-stable
3106	GROMACS	Task	New	Normal	Implement multiple pulses with GPU communication	Alan Gray	09/25/2019 02:23 PM	
3105	GROMACS	Task	New	Normal	implement GPU PME/PP comm cycle counting		09/24/2019 03:19 PM	2020
3104	GROMACS	Task	New	Normal	implement GPU DD cycle counting		09/24/2019 03:19 PM	2020
3097	GROMACS	Bug	New	Normal	nbnxm grid issue with regressiontest complex/nbnxn_rzero with gpubufferops path		09/24/2019 03:26 PM	2020-beta2
3096	GROMACS	Task	New	Normal	Multiple time-stepping: correct coupling algorithms, virial calculation and energy output	Christian Blau	09/18/2019 02:18 PM	2021-infrastructure-stable
3093	GROMACS	Task	New	High	rework GPU direct halo-exchange related force reduction complexities		10/11/2019 05:53 PM	2020
3092	GROMACS	Task	New	Normal	implement better receiver ready / notify in halo exchange		09/18/2019 02:47 AM	2020
3088	GROMACS	Bug	New	Normal	Reference to theory needed for cylindrical pull geometry		09/13/2019 11:26 AM	
3087	GROMACS	Feature	New	Normal	enable GPU peer to peer access		09/12/2019 04:24 PM	2020

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
3086	GROMACS	Bug	New	Normal	gmxapi fails with MPI build of GROMACS 2020		09/25/2019 04:18 PM	
3083	GROMACS	Bug	New	Normal	Listed forces tests failing on ICC19 with AVX2_256 nightly build		09/10/2019 11:56 AM	
3082	GROMACS	Task	New	High	move launch/synchronization points to clarify task dependencies		10/11/2019 05:53 PM	2020
3078	GROMACS	Task	New	Normal	Allow MD modules to register energy output fields themselves		09/06/2019 11:36 AM	
3077	GROMACS	Task	New	Normal	PME/PP GPU Comms unique pointer deletion causes seg fault when CUDA calls exist in destructor		09/20/2019 01:04 PM	
3076	GROMACS	Task	New	Normal	Selectively activate MdModules during simulation instead of instantiating all of them	Christian Blau	09/05/2019 11:36 AM	2021-infrastructure-stable
3075	GROMACS	Bug	New	Normal	Frozen atoms are moving		09/04/2019 08:00 PM	
3073	GROMACS	Bug	New	Normal	Total potential energy goes crazy, but I don't know why this happens.		09/04/2019 07:25 PM	
3072	GROMACS	Task	New	Normal	Use gmx::index for indexing instead of int	Christian Blau	09/03/2019 04:23 PM	2021-infrastructure-stable
3069	GROMACS	Feature	New	Low	Iterator over span and indices into this span (zip-style iterator)	Christian Blau	08/29/2019 11:11 AM	future
3068	GROMACS	Bug	New	Normal	Misleading warning on rerun		08/26/2019 03:44 PM	
3066	GROMACS	Bug	New	Normal	Gauss transform and density fit classes should operate on real values instead of float	Christian Blau	08/26/2019 11:53 AM	
3064	GROMACS	Task	New	Normal	add test for perturbed bonded forces		08/22/2019 06:34 PM	2020
3062	GROMACS	Task	New	Normal	add twin cut-off mdrun test		08/19/2019 06:21 PM	2020
3057	GROMACS	Task	New	Normal	re-enable fusion on Power8/9	Szilárd Páll	08/12/2019 11:41 AM	2020
3054	GROMACS	Bug	New	Normal	Missing dihedral define		08/02/2019 05:47 PM	
3052	GROMACS	Feature	New	Normal	GPU virial reduction/calculation		08/01/2019 05:26 PM	
3050	GROMACS	Bug	New	Low	Fix tests on Solaris	Vedran Miletic	07/29/2019 12:38 PM	2020
3049	GROMACS	Bug	New	Low	gmx nmeig should plot a real infrared spectrum	David van der Spoel	09/24/2019 03:25 PM	future
3048	GROMACS	Bug	New	Normal	Dihedral parameters for N-terminal in gromos53a6 force field in the aminoacids.n.tdb file with different values in versions 4.6.7 and gromacs 2019/2016/5.1.5		07/29/2019 10:41 AM	
3047	GROMACS	Task	New	Normal	Set required versions for GROMACS 2021		08/24/2019 05:25 PM	2021-infrastructure-stable
3045	GROMACS	Feature	New	Low	Option to remove v-sites in trjconv?		07/19/2019 04:42 PM	
3042	GROMACS	Bug	New	Normal	core dump error in grompp command		10/09/2019 07:30 PM	
3041	GROMACS	Task	New	Normal	Remove workaround for gcc bug 58265		07/23/2019 12:27 PM	
3040	GROMACS	Task	New	Normal	Refactor Restraint module		07/18/2019 03:59 PM	

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
3038	GROMACS	Feature	New	Normal	Improvements to MD plugin development environment	Eric Irrgang	07/17/2019 02:15 PM	2020
3037	GROMACS	Task	New	Normal	add missing cycle counters related to buffer ops/reduction launches		09/24/2019 03:27 PM	2020
3035	GROMACS	Task	New	Normal	Provide central logger in wrapper binary	Paul Bauer	09/06/2019 02:34 PM	2021-infrastructure-stable
3032	GROMACS	Feature	New	Normal	Clean up dev-manual structure		07/11/2019 11:48 AM	2020
3031	GROMACS	Task	New	Normal	evaluate the impact of particle order on PME		08/21/2019 06:08 PM	2020
3030	GROMACS	Feature	New	Normal	RST style guidelines		07/09/2019 03:38 PM	
3026	GROMACS	Task	New	Normal	add flags for GPU force buffer op / reduction activation		08/01/2019 04:46 PM	2020
3024	GROMACS	Bug	New	Normal	Bad logic for Sphinx detection CMake output		07/05/2019 05:44 PM	2020
3022	GROMACS	Feature	New	Normal	modernized naming for new GPU developments		07/04/2019 10:48 AM	2020
3021	GROMACS	Feature	New	Normal	Completion of docs for GPU developments		07/04/2019 10:45 AM	2020
3020	GROMACS	Feature	New	Low	modernize DeviceBuffer and GPU memory management		08/13/2019 06:01 PM	
3017	GROMACS	Bug	New	Normal	ddBalanceRegionHandler triggers need fixing		09/24/2019 03:25 PM	2020-beta2
3016	GROMACS	Task	New	Normal	intermittent failure of essentialdynamics test		07/18/2019 05:23 PM	
3015	GROMACS	Task	New	Normal	Create central log handle for calls to gmxfatal		09/06/2019 02:34 PM	2021-infrastructure-stable
3014	GROMACS	Task	New	Normal	gmxfapi example Python scripts		06/28/2019 11:07 AM	2020
3013	GROMACS	Task	New	Normal	Extend logging levels in MDLogger		09/06/2019 02:34 PM	2021-infrastructure-stable
3008	GROMACS	Task	New	Normal	verify block size choice of CUDA bonded kernel		06/26/2019 08:38 PM	2020
3005	GROMACS	Task	New	Normal	Move logging in gmxf preprocess to MDLogger		06/26/2019 10:01 AM	
3004	GROMACS	Task	New	Normal	Move trajectory analysis logging to MDLogger		06/26/2019 09:59 AM	
3003	GROMACS	Task	New	Normal	implement heuristic fallback to CPU when there is too little work for GPU offload		06/25/2019 04:10 PM	
3002	GROMACS	Task	New	Normal	consider splitting bonded work into local/nonlocal		06/25/2019 04:06 PM	
3001	GROMACS	Task	New	Normal	explore simplifying virial and shift force reduction		06/25/2019 04:03 PM	2020
3000	GROMACS	Bug	New	Normal	CMake "webpage" target does not fail when it should		06/25/2019 02:43 PM	
2999	GROMACS	Task	New	Normal	Move all logging in core library and tools to use MDLogger		09/06/2019 02:36 PM	2021-infrastructure-stable
2997	GROMACS	Task	New	Normal	improve performance of alchemical free energy calculations		06/24/2019 03:07 PM	2020
2996	GROMACS	Feature	New	Normal	gmxfapi execution model	Eric Irrgang	06/24/2019 02:16 PM	2020
2994	GROMACS	Feature	New	Normal	Data flow topology in gmxfapi 2020		06/24/2019 01:53 PM	2020
2993	GROMACS	Feature	New	Normal	Scalar and structured type expression and definitions for API	Eric Irrgang	10/17/2019 09:55 AM	
2992	GROMACS	Task	New	Normal	Split hw_opt in const user options and dynamic settings		09/24/2019 03:23 PM	2020
2990	GROMACS	Bug	New	Normal	ARM neon SIMD4 error		09/24/2019 03:25 PM	2020-beta2

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
2987	GROMACS	Bug	New	Normal	assess the bonded GPU task assignment default		10/21/2019 04:15 PM	2020
2985	GROMACS	Feature	New	Normal	Python package documentation		06/19/2019 12:24 PM	2020
2984	GROMACS	Feature	New	Normal	More Extensive Selections Examples	Dallas Warren	06/18/2019 11:50 PM	
2983	GROMACS	Task	New	Normal	better suited data-types for bonded GPU kernels		07/11/2019 04:32 PM	
2981	GROMACS	Bug	New	Normal	segfault in opencl build		06/18/2019 03:30 AM	
2980	GROMACS	Bug	New	Normal	taskassignment fails with unit tests when GPUs and custom number of ranks is used		06/17/2019 05:28 PM	
2978	GROMACS	Bug	New	Normal	Some suggestions about the gmx current tool		06/13/2019 12:41 PM	
2977	GROMACS	Feature	New	Normal	print DD load balancing improvement		06/13/2019 10:56 AM	
2976	GROMACS	Task	New	Normal	Basic math for Multidimensional arrays		08/04/2019 09:44 PM	2020
2975	GROMACS	Feature	New	Normal	LJ PME calculations on GPUs		06/12/2019 01:17 PM	
2974	GROMACS	Bug	New	Normal	position-restraints regressiontest fails on intel GPU		10/01/2019 11:12 AM	2019.5
2967	GROMACS	Feature	New	Normal	GPU reallocateDeviceBuffer improvements		09/24/2019 06:52 PM	2020-beta2
2965	GROMACS	Task	New	Normal	Performance of GPU direct communications		05/31/2019 03:12 PM	2020
2961	GROMACS	Feature	New	Normal	How should Python package find GROMACS resources under various circumstances?		10/02/2019 02:06 PM	
2958	GROMACS	Bug	New	Normal	Compiling master (to become 2020) using CUDA 9.0		10/14/2019 09:15 PM	2020-beta2
2957	GROMACS	Feature	New	Normal	add support for the Hygon Dhyana architecture		05/21/2019 01:00 PM	2020
2956	GROMACS	Feature	New	Normal	SAXS resolution		05/17/2019 09:58 AM	
2954	GROMACS	Bug	New	Normal	genion changes residue numbering		05/26/2019 12:08 AM	
2949	GROMACS	Bug	New	Normal	cmake fails when building mdrun only		07/08/2019 10:04 AM	
2948	GROMACS	Bug	New	Normal	SIMD support detected as none on AMD R5 2500U		05/21/2019 12:58 PM	
2945	GROMACS	Task	New	Normal	Give MdModules access to simulation resources (e.g. atom selection manager or communication infrastructure)	Christian Blau	05/19/2019 01:26 PM	2020
2944	GROMACS	Feature	New	Normal	Roadmap for thermostats / barostats in new propagation/integration scheme	Michael Shirts	05/08/2019 05:50 PM	2020
2943	GROMACS	Task	New	Normal	Rename Integrator	Pascal Merz	05/23/2019 08:04 PM	2020
2936	GROMACS	Task	New	Normal	introduce check that CPU-GPU transfers are made between arrays of compatible types		05/13/2019 09:23 AM	2020
2934	GROMACS	Feature	New	Normal	GPU X Buffer ops		09/24/2019 06:07 PM	2020
2933	GROMACS	Task	New	Normal	Convert walls to a ForceProvider		04/25/2019 02:43 PM	
2931	GROMACS	Feature	New	Normal	Tables in Verlet kernels		04/29/2019 12:01 PM	
2930	GROMACS	Feature	New	Normal	Limited range for reference group detection in cylinder pulling		04/26/2019 05:17 PM	

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
2928	GROMACS	Feature	New	Normal	Add ability to use expression "count of ATOM_EXPR" in selection statements.		04/16/2019 04:52 PM	
2925	GROMACS	Bug	New	Normal	BasicVector addition operator yields unexpected result when adding scalar	Christian Blau	04/20/2019 05:39 PM	2020
2924	GROMACS	Bug	New	Normal	Failing version check when reading new tpr file with older gromacs version		04/12/2019 10:52 AM	
2919	GROMACS	Task	New	Normal	C++ style guidelines for namespace use		04/15/2019 01:21 PM	
2916	GROMACS	Task	New	Normal	Decide future of symtab	Paul Bauer	09/06/2019 02:35 PM	2021-infrastructure-stable
2915	GROMACS	Feature	New	High	GPU direct communications		10/11/2019 05:53 PM	
2910	GROMACS	Feature	New	Normal	Mixed scaling for 1-4 interactions		04/10/2019 10:13 PM	
2909	GROMACS	Task	New	Normal	consider implementing mechanisms to ensure pair lists are not used past their max lifetime		04/03/2019 05:14 PM	
2908	GROMACS	Task	New	Normal	Renaming things in nbxnm	Berk Hess	03/28/2019 10:10 AM	
2907	GROMACS	Bug	New	Normal	Gromacs autocompletion appears to be broken with ZSH		07/16/2019 04:46 AM	
2905	GROMACS	Task	New	Normal	Add a Jenkins configuration with std library assert		08/24/2019 05:22 PM	
2902	GROMACS	Bug	New	Normal	2019.1 equilibration issue? (Intel 2018u3)		04/30/2019 08:17 AM	
2901	GROMACS	Feature	New	Normal	Declare external Resources in mdp / tpr files.	Christian Blau	03/27/2019 04:27 PM	2020
2898	GROMACS	Task	New	Low	Naming common variables		03/26/2019 11:46 PM	
2897	GROMACS	Bug	New	Normal	rotation/flex2 can still fail on cpu-only run on OpenCL build		04/04/2019 06:24 PM	
2891	GROMACS	Feature	New	High	PME/PP GPU communications		10/17/2019 02:57 PM	
2890	GROMACS	Feature	New	High	GPU Halo Exchange		10/17/2019 02:00 PM	2020
2889	GROMACS	Task	New	Normal	update grompp warnings for brevity, usefulness and actionability	Mark Abraham	03/11/2019 02:15 PM	2020
2888	GROMACS	Feature	New	High	CUDA Update and Constraints module	Artem Zhmurov	10/21/2019 03:59 PM	2020
2887	GROMACS	Feature	New	Normal	CUDA version of Leap Frog algorithm	Artem Zhmurov	10/02/2019 12:00 PM	2020
2886	GROMACS	Feature	New	Normal	CUDA version of SETTLE	Artem Zhmurov	10/02/2019 12:02 PM	2020
2885	GROMACS	Feature	New	Normal	CUDA version of LINCS	Artem Zhmurov	03/12/2019 01:33 PM	2020
2883	GROMACS	Bug	New	Normal	essentialdynamics fail with Intel MPI		03/08/2019 03:10 AM	
2882	GROMACS	Task	New	Normal	evaluate different storage layouts for GPU coordinates/changes/forces	Szilárd Páll	03/07/2019 06:21 PM	
2877	GROMACS	Task	New	Normal	use gmx::Options more	Mark Abraham	04/02/2019 06:14 PM	2020
2876	GROMACS	Bug	New	Normal	2019.1 make check fails on AVX and AVX2 (Intel 2018u3)	Erik Lindahl	03/08/2019 10:32 AM	

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
2874	GROMACS	Task	New	Normal	Refactor Gromacs (cluster) neighborlist into separate module	Erik Lindahl	02/28/2019 11:36 AM	
2873	GROMACS	Bug	New	Normal	Simple way to get last frame from trajectory		02/28/2019 11:14 PM	
2872	GROMACS	Bug	New	Normal	gmx solvate and genion topology update		02/27/2019 10:18 AM	
2870	GROMACS	Bug	New	Normal	GPU detection error message missing from the output		03/05/2019 03:55 PM	
2869	GROMACS	Bug	New	Normal	GPU detection error only issued as a note to the log		03/05/2019 04:09 PM	
2866	GROMACS	Feature	New	Normal	Alternative non-bonded potentials	David van der Spoel	03/05/2019 03:50 PM	future
2864	GROMACS	Task	New	Normal	Building incompatibilities	Benson Muite	02/19/2019 02:00 PM	
2863	GROMACS	Task	New	Normal	improve PBC handling		03/11/2019 04:28 PM	
2860	GROMACS	Feature	New	Normal	Option for outputting min/max coordinates in gmx traj		02/08/2019 12:35 AM	
2857	GROMACS	Task	New	Normal	Clarify recommended function specifies (constexpr, noexcept, pure)		02/04/2019 04:48 AM	
2855	GROMACS	Task	New	Normal	Allow compiling GROMACS without C compiler		01/31/2019 08:44 PM	
2854	GROMACS	Bug	New	Normal	OnlineHelpUnitTests segfaults on s390x with gcc-9.0.1	Paul Bauer	02/04/2019 11:17 AM	
2853	GROMACS	Bug	New	Normal	EwaldUnitTests segfault on armv7hl with gcc-9.0.1	Paul Bauer	02/04/2019 05:34 PM	
2852	GROMACS	Bug	New	Low	the in-tree regressiontest download can get out of sync with code		01/30/2019 03:58 PM	
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	
2846	GROMACS	Feature	New	Low	Set rpath in FindLibStdCpp.cmake		02/02/2019 08:09 AM	
2840	GROMACS	Feature	New	Normal	Test that functionality does not compile that is not supposed to.		01/25/2019 02:35 PM	future
2839	GROMACS	Task	New	Normal	make module and file naming consistent		04/09/2019 04:27 PM	2020
2835	GROMACS	Task	New	Normal	Matrix class constraint to upper or lower triangle		02/07/2019 02:44 PM	
2834	GROMACS	Task	New	Normal	C++ matrix classes	Christian Blau	01/23/2019 12:19 PM	2020
2833	GROMACS	Task	New	Normal	Update topology datastructures	Paul Bauer	04/02/2019 12:39 PM	2020
2832	GROMACS	Bug	New	Low	PaddedVector move operations broken	Mark Abraham	02/12/2019 03:22 PM	2020
2831	GROMACS	Task	New	Normal	Bump required version numbers of infrastructure for 2020	Mark Abraham	08/23/2019 03:24 PM	2020-infrastructure-update-post-beta1
2816	GROMACS	Feature	New	High	GPU offload / optimization for update&constraints, buffer ops and multi-gpu communication	Alan Gray	10/14/2019 01:32 PM	2020
2806	GROMACS	Feature	New	Normal	SIMD algorithms for ARM SVE // nobonded cluster and others		12/12/2018 05:52 PM	2020
2798	GROMACS	Bug	New	Normal	Default mpi rank number fails when there are 16 cores and 3 gpus	Berk Hess	12/11/2018 10:11 PM	2020

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
2796	GROMACS	Task	New	Low	clarify what mdrun -cpt means		01/03/2019 02:09 PM	
2795	GROMACS	Task	New	Normal	Incorporate regressiontests into core gromacs		02/13/2019 08:17 PM	2020
2792	GROMACS	Task	New	Normal	Improvement of PME gather and spread CUDA kernels		09/12/2019 12:23 PM	
2788	GROMACS	Bug	New	Normal	PME will not run on AMD GPU with NVidia GPU present		01/03/2019 02:24 PM	
2787	GROMACS	Task	New	Normal	allow passing flags to allocateDeviceBuffer		12/03/2018 01:54 PM	
2785	GROMACS	Bug	New	Normal	Inconsistent and erroneous behaviour of trjconv when writing a partial TNG		11/30/2018 02:36 PM	
2774	GROMACS	Feature	New	Normal	Refactor shell code into its own integrator	David van der Spoel	03/29/2019 05:20 PM	2020
2773	GROMACS	Task	New	Normal	improve GPU error handling and make such handling uniform across modules		11/21/2018 10:28 AM	2020
2771	GROMACS	Task	New	Normal	Size independent Hessian for normal mode analysis		12/08/2018 08:06 PM	2020
2770	GROMACS	Task	New	Normal	change branch maintenance policy		11/29/2018 02:51 PM	2020
2767	GROMACS	Bug	New	Normal	grompp warns about md + FEP even for fully coupled states		11/19/2018 11:41 AM	2020
2764	GROMACS	Task	New	Normal	gmxapi version updates for post release-2019	Eric Irrgang	11/21/2018 12:53 PM	
2763	GROMACS	Bug	New	Normal	GMXAPI layout / grouping in development docs "modules" page		12/14/2018 12:49 PM	future
2761	GROMACS	Feature	New	Low	lincs-order 4 is too conservative for some force fields		11/16/2018 09:55 AM	
2758	GROMACS	Task	New	Low	Modernize genconf		11/15/2018 07:38 AM	future
2755	GROMACS	Feature	New	Low	md5 sums and sha256, sha512 hashes	Benson Muite	02/19/2019 11:00 PM	
2754	GROMACS	Bug	New	Normal	Simulated Tempering seems to be broken	Michael Shirts	02/05/2019 03:58 PM	
2740	GROMACS	Bug	New	Normal	mdrun reports incorrect error with -bonded gpu without gpu	Mark Abraham	11/07/2018 01:59 PM	
2739	GROMACS	Feature	New	Normal	Parallel continuous tempering and enhanced sampling feature		11/13/2018 11:36 PM	
2735	GROMACS	Task	New	Normal	Allow gmx_genrestr to write correct position restraints for molecules after the first molecule	Joe Jordan	11/09/2018 12:19 PM	2020
2730	GROMACS	Task	New	Normal	Add tests for gmx_genion	Joe Jordan	11/02/2018 06:42 PM	2020
2728	GROMACS	Bug	New	Normal	Fix NB kernel picking		11/02/2018 03:51 PM	2020
2723	GROMACS	Task	New	Normal	Update mdrun-performance.rst to clearly express the nature of task	Joe Jordan	10/21/2019 04:13 PM	2020
2722	GROMACS	Bug	New	Normal	gmxapi may over-manage RPATH	Mark Abraham	10/16/2019 10:28 AM	2020-beta3
2715	GROMACS	Feature	New	Normal	Avoid requesting the user to recompile gromacs for Intel OpenCL support		10/31/2018 12:16 PM	2020
2713	GROMACS	Feature	New	Normal	Constant offset for external electric fields		10/28/2018 12:57 AM	

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
2710	GROMACS	Feature	New	Normal	Separate dvdI for each molecule (of couple-moltype) when running FEP		10/26/2018 10:24 AM	2020
2707	GROMACS	Bug	New	Normal	Installed OpenCL files include clh file from gpu_utils directory		10/30/2018 04:02 AM	
2699	GROMACS	Task	New	Normal	Test POWER9		04/05/2019 04:50 PM	2020
2698	GROMACS	Task	New	Normal	gmxapi documentation integration		03/02/2019 01:31 AM	
2697	GROMACS	Task	New	Normal	improve FFT library flavor/version reporting		12/10/2018 01:49 PM	2020
2695	GROMACS	Task	New	Low	bonded GPU module timing		01/21/2019 01:19 PM	2020
2693	GROMACS	Bug	New	Normal	Several memory leaks in mdrun		12/18/2018 04:22 AM	future
2686	GROMACS	Task	New	Normal	add tests for gpu bonded interactions		11/29/2018 10:44 AM	2020
2682	GROMACS	Task	New	Normal	Add MSAN configuration		10/09/2018 06:28 PM	
2672	GROMACS	Task	New	Normal	check & document execution width requirements in OpenCL		12/31/2018 11:20 AM	future
2671	GROMACS	Task	New	Normal	replace constants like M_PI		10/05/2018 08:58 AM	2020
2670	GROMACS	Task	New	Low	remove old/backward compatibility OpenCL support from releng		10/04/2018 06:06 PM	
2667	GROMACS	Feature	New	Normal	Suggested steps for calculating entropy in solution and binding	David van der Spoel	10/30/2018 02:06 PM	2020
2660	GROMACS	Task	New	Low	rework OpenCL nbxn kernel constants	Szilárd Páll	10/30/2018 12:10 PM	2020
2658	GROMACS	Task	New	Normal	Secondary structure assignment via DSSP as native gromacs code	Christian Blau	10/09/2018 04:51 PM	future
2657	GROMACS	Bug	New	Normal	Biphasic tutorial		09/28/2018 10:02 AM	
2650	GROMACS	Task	New	Normal	revise OpenCL stack recommendations		12/31/2018 11:19 AM	future
2649	GROMACS	Bug	New	Normal	Virial calculation necessary for correct energy calculation on GPU		12/17/2018 02:32 PM	future
2645	GROMACS	Bug	New	Normal	Security		09/28/2018 01:16 PM	
2644	GROMACS	Task	New	Normal	Replace compute_globals	Mark Abraham	09/24/2018 05:51 PM	future
2643	GROMACS	Feature	New	Low	mdp options and/or docs for anisotropic aspects of implementations		09/12/2018 02:23 PM	
2637	GROMACS	Bug	New	High	gmx solvate tears apart molecules		09/11/2018 07:43 PM	
2632	GROMACS	Task	New	Low	make sure cmake defines proper hwloc version with cross-compilation enabled		12/03/2018 01:35 PM	future
2624	GROMACS	Bug	New	Normal	GPU build system not robust enough		09/05/2018 02:00 AM	
2622	GROMACS	Feature	New	Low	Reduce severity of Berendsen warning		08/23/2018 11:16 PM	future
2621	GROMACS	Task	New	Normal	Fine-Grained API to Describe Force Calculation and Neighbourhood Search	Prashanth Kanduri	08/22/2018 11:36 AM	future

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
2616	GROMACS	Task	New	Normal	Model for MD state		09/14/2018 05:12 PM	
2611	GROMACS	Bug	New	Normal	issues with gpu_utils-test with GMX_BUILD_UNITTESTS=OFF and on OSX		08/14/2018 07:03 PM	
2608	GROMACS	Task	New	Normal	Remove code duplication between OpenCL and CUDA		09/24/2018 12:47 PM	
2607	GROMACS	Bug	New	Normal	Grompp becomes extremely slow when many pull groups are present		08/11/2018 08:54 AM	
2606	GROMACS	Bug	New	Normal	Free Energy Calculation -- Function type Fourier Dih. Not implemented in ip_pert		08/10/2018 01:48 AM	
2603	GROMACS	Task	New	Normal	Add ability to properly check coordinate files during testing	Paul Bauer	10/15/2018 01:16 PM	future
2602	GROMACS	Bug	New	Low	build information gets outdated if build tree is reused		08/13/2018 09:04 PM	
2601	GROMACS	Feature	New	Normal	Free energy calculations, soft-core potential	Vytautas Gapsys	03/05/2019 01:44 AM	future
2600	GROMACS	Bug	New	High	coul-lambdas turns off all coulombic interactions in system instead of the molecule specified in the couple-moltype		08/07/2018 06:50 PM	
2598	GROMACS	Bug	New	Normal	Tools using read_next_x cannot read TNG files with sanitizers		10/15/2018 01:16 PM	future
2596	GROMACS	Feature	New	Normal	Constant potential method	Benson Muite	05/10/2019 09:54 AM	
2595	GROMACS	Task	New	Normal	Reusable Utilities for Schedules	Prashanth Kanduri	02/22/2019 03:48 PM	future
2594	GROMACS	Feature	New	Normal	Multi-level GMX API	Prashanth Kanduri	02/22/2019 03:48 PM	future
2590	GROMACS	Task	New	Normal	Essential Dynamics as module providing forces	Christian Blau	08/22/2018 05:03 PM	future
2579	GROMACS	Feature	New	Normal	Add dimensionality option to gmx trjconv -center		07/19/2018 04:53 PM	future
2576	GROMACS	Bug	New	Normal	gmx potential -correct outputs the wrong potential		07/25/2018 02:58 PM	
2574	GROMACS	Feature	New	Normal	iForceSchedule Abstraction	Prashanth Kanduri	03/29/2019 05:20 PM	future
2573	GROMACS	Bug	New	High	Different mdp files describing the same change yield different free energy on the same trajectory		07/19/2018 06:52 PM	
2570	GROMACS	Feature	New	Normal	Better string formatting and printing		05/02/2019 12:20 PM	
2568	GROMACS	Bug	New	Low	gmx editconf -rotate does not rotate the box		07/10/2018 10:27 AM	future
2567	GROMACS	Bug	New	Normal	make check fails at test 23 SIMD errors		07/10/2018 09:35 AM	
2564	GROMACS	Bug	New	Normal	Result Summary Different For Jobs With Different Numbers of Nodes		07/05/2018 02:39 PM	
2563	GROMACS	Bug	New	Normal	Windows 7 Compilation with GPU support		07/02/2018 09:58 AM	
2556	GROMACS	Feature	New	Normal	make default selections suitable for DNA and RNA	Mark Abraham	06/20/2018 01:48 PM	
2555	GROMACS	Bug	New	Low	building GROMACS 2018.2		07/03/2018 11:41 PM	

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
2547	GROMACS	Feature	New	Low	Add option of averaging and obtaining error bars for AWH PMFs	Viveca Lindahl	06/06/2018 11:31 AM	future
2546	GROMACS	Task	New	Normal	Add more assertions to AWH code	Viveca Lindahl	06/06/2018 11:20 AM	future
2545	GROMACS	Feature	New	Normal	Should grompp fix periodicity of input files?	David van der Spoel	10/03/2018 11:32 PM	future
2544	GROMACS	Bug	New	Normal	gmx rmsf does not fix periodicity in reference structure	David van der Spoel	08/21/2018 10:36 AM	future
2538	GROMACS	Task	New	Normal	organize more of the PME GPU code along task-specific lines	Mark Abraham	05/31/2018 05:41 PM	
2537	GROMACS	Task	New	Normal	Simplify PME solve reduction	Aleksei lupinov	10/30/2018 12:08 PM	2020
2535	GROMACS	Task	New	Normal	consider compiling opencl fft kernels once		05/31/2018 01:33 PM	
2532	GROMACS	Task	New	Normal	enable queue priorities in OpenCL		05/29/2018 02:29 PM	
2531	GROMACS	Task	New	Low	Consider optimizing tabulated data access on GPU		07/30/2018 12:31 PM	
2530	GROMACS	Task	New	Normal	consider using CUDA Driver API		09/23/2018 11:47 PM	future
2528	GROMACS	Task	New	Normal	PME GPU tuning		12/31/2018 11:18 AM	future
2527	GROMACS	Task	New	Normal	Rename GpuEventSynchronizer to something more fitting (after mergin PME OpenCL)		10/30/2018 04:06 AM	future
2526	GROMACS	Bug	New	Normal	Bug of gmx hbond		05/30/2018 03:12 PM	
2524	GROMACS	Task	New	Normal	struct alignment/packing for OpenCL host & device code		10/30/2018 12:06 PM	2020
2522	GROMACS	Task	New	Normal	OpenCL context duplication		10/30/2018 12:07 PM	2020
2521	GROMACS	Task	New	Normal	Implement alternating PME/NB wait for OpenCL		10/15/2018 12:39 PM	
2520	GROMACS	Task	New	Normal	Treat OpenCL kernel width more diligently		05/24/2018 06:21 PM	
2519	GROMACS	Task	New	High	Improve/remove PME OpenCL kernel barriers		02/15/2019 06:34 PM	
2518	GROMACS	Task	New	Normal	redesign task-assignment code for OpenCL		12/28/2018 12:38 PM	2020
2516	GROMACS	Task	New	Low	Support PME OpenCL execution width < 16	Aleksei lupinov	06/05/2019 05:32 PM	
2514	GROMACS	Task	New	Normal	PME OpenCL reductions with intrinsics		05/31/2018 12:27 AM	future
2501	GROMACS	Task	New	Normal	Documentation section on log file contents	Kevin Boyd	10/03/2018 09:48 PM	future
2498	GROMACS	Task	New	Normal	OpenCL memory pinning/mapping		10/30/2018 12:07 PM	2020
2496	GROMACS	Task	New	Low	find system xdr properly		05/02/2018 02:19 PM	
2495	GROMACS	Task	New	Normal	replace -noconfout with mdp option	Mark Abraham	10/12/2018 10:34 PM	2020
2492	GROMACS	Task	New	Normal	implement force calculation via ForceProviders containing collections of IForceProvider	Mark Abraham	09/19/2018 03:13 PM	future

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
2491	GROMACS	Feature	New	Low	Allow constant bias AWH simulations	Viveca Lindahl	06/05/2018 10:38 PM	future
2490	GROMACS	Task	New	Normal	evaluate two-step communicators	Szilárd Páll	10/03/2018 09:47 PM	future
2488	GROMACS	Task	New	Normal	use MPI non-blocking collectives to overlap pull comm		04/25/2018 04:19 PM	
2483	GROMACS	Bug	New	Low	gmx dump writes mdp files that can not be parsed by grompp	Paul Bauer	10/08/2018 10:50 AM	future
2481	GROMACS	Task	New	Low	Update gmx report-methods to write more method information		09/20/2018 07:43 AM	2020
2480	GROMACS	Bug	New	Normal	pdb2gmx does not protonate correctly for united-atom Gromos	Mark Abraham	12/17/2018 01:27 PM	2020
2478	GROMACS	Task	New	Low	avoid use of getenv in static initialization		04/13/2018 11:57 AM	
2475	GROMACS	Task	New	Normal	make OpenCL 1st class-citizen in the build system		10/30/2018 12:01 PM	2020
2473	GROMACS	Bug	New	Normal	mdrun sometimes stalls due to large coordinates with no constraints		04/04/2018 10:15 PM	
2469	GROMACS	Task	New	Normal	implement GPU timer reduction for reporting		03/27/2018 05:08 PM	
2468	GROMACS	Bug	New	Low	incorrect GPU timing reported with OpenCL and domain decomposition		12/17/2018 01:28 PM	future
2464	GROMACS	Task	New	Normal	GPU performance goals overview		03/26/2018 10:42 AM	
2463	GROMACS	Task	New	Low	PME GPU decomposition		03/26/2018 10:42 AM	
2462	GROMACS	Task	New	Normal	consider adding STL misuse tests		03/23/2018 01:23 AM	
2460	GROMACS	Bug	New	Normal	Allow inclusion of user libraries through CMake cache variables		03/28/2018 08:47 PM	
2456	GROMACS	Task	New	Normal	Add a pull module external potential tests		03/15/2018 03:02 PM	
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	
2442	GROMACS	Task	New	Normal	Port gmx saxs and gmx sans to c++	Joe Jordan	06/28/2018 10:06 PM	future
2435	GROMACS	Task	New	Normal	identify and note about/tune task offload in GPU-bound runs		03/02/2018 04:08 PM	
2429	GROMACS	Feature	New	Normal	Add option of periodic chain topology to pdb2gmx		03/10/2018 01:01 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	
2427	GROMACS	Bug	New	Normal	gmx select gives syntax error for selection involving evaluating simple arithmetic expression		02/27/2018 05:15 PM	
2425	GROMACS	Task	New	Normal	testing multisim with multiple ranks per simulation	Mark Abraham	11/29/2018 11:20 AM	2020
2423	GROMACS	Task	New	Normal	modernize constraints code	Mark Abraham	09/19/2018 03:01 PM	future
2422	GROMACS	Task	New	Normal	write C kernel for tables in Verlet scheme		02/26/2018 01:38 PM	

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
2412	GROMACS	Task	New	Normal	attempt to do better FFTW planning		03/15/2018 05:01 PM	
2402	GROMACS	Task	New	Normal	PME kernels general performance improvements		03/26/2018 10:41 AM	future
2396	GROMACS	Task	New	Normal	Refactor trajectoryanalysis module to allow handling of trajectory frame manipulation	Paul Bauer	10/08/2018 07:29 PM	2020
2393	GROMACS	Bug	New	Normal	incorrect error message with omitted command line flag before its argument		01/24/2018 11:24 PM	
2383	GROMACS	Task	New	Normal	Add JSON interface to write and read files	Paul Bauer	01/16/2018 02:01 PM	future
2382	GROMACS	Task	New	Normal	Simplify Doxygen guidelines		01/13/2018 12:40 AM	
2380	GROMACS	Bug	New	Low	cycle counter issues with separate PME rank + GPUs		01/16/2018 10:21 PM	
2379	GROMACS	Task	New	Normal	check leftover FIXMEs in r2018	Szilárd Páll	12/31/2018 11:16 AM	future
2376	GROMACS	Task	New	Normal	max_mpi_ranks has wrong name		02/10/2018 11:03 AM	
2375	GROMACS	Task	New	Normal	Clarify execution phases for MD simulation		04/30/2019 12:59 PM	
2373	GROMACS	Bug	New	Low	gmx -nice can't work		01/04/2018 11:17 AM	
2371	GROMACS	Task	New	Normal	mtop searching needs reconsideration		01/04/2018 11:54 AM	future
2367	GROMACS	Task	New	Normal	construct pbc_simd less often		09/24/2018 11:02 PM	future
2360	GROMACS	Bug	New	Low	error at counter reset with PME-only rank		01/05/2018 12:43 PM	future
2354	GROMACS	Feature	New	Normal	develop configuration file support for control of task layout		09/19/2018 03:01 PM	future
2353	GROMACS	Task	New	Normal	improve on relative tolerance for constructing tables		10/30/2018 04:17 AM	2020
2351	GROMACS	Task	New	Normal	Avoid the SIMD module depending on non-trivial parts of Gromacs		12/14/2017 02:47 AM	future
2341	GROMACS	Task	New	Low	assess the state of building and using GROMACS on Windows		07/29/2019 11:09 PM	future
2304	GROMACS	Task	New	Normal	Document and propose tracking mdrun heuristics		10/03/2018 09:39 PM	future
2294	GROMACS	Task	New	Normal	Require identical hardware on nodes on parallel runs		11/19/2017 08:54 PM	
2289	GROMACS	Feature	New	Normal	gmx spatial add ability to perform over multiple reference structures		11/08/2017 12:31 AM	
2283	GROMACS	Feature	New	Normal	Force distribution analysis	Bernd Doser	10/27/2017 11:44 AM	
2282	GROMACS	Feature	New	Normal	Density map toolset	Christian Blau	03/21/2019 06:08 PM	future
2255	GROMACS	Bug	New	Normal	nstlist override stopped affecting the input parameter listing		12/17/2017 08:05 AM	
2254	GROMACS	Feature	New	Normal	GPU extensions for Google Tests		09/19/2017 05:01 PM	
2252	GROMACS	Bug	New	Low	Memory allocation failures with large page sizes during PME tuning		12/14/2017 04:27 AM	
2248	GROMACS	Feature	New	Normal	Label all SIMD functions as pure/nodiscard		02/04/2019 04:49 AM	
2241	GROMACS	Bug	New	Low	refdata can segfault when reading		09/07/2017 11:57 AM	
2239	GROMACS	Feature	New	Normal	split libgromacs into base and full		01/07/2019 01:47 AM	

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
2232	GROMACS	Bug	New	Normal	pdb2gmx can't form special bonds with terminal patched atoms		12/03/2017 01:35 PM	
2231	GROMACS	Bug	New	Normal	convert-tpz aborts when saving subset of the system		01/12/2018 03:52 PM	
2229	GROMACS	Feature	New	High	Full Object Oriented Modularization of GROMACS MDRUN Codebase	Mark Abraham	08/22/2018 05:03 PM	future
2226	GROMACS	Feature	New	Normal	Harmonise commands for exit in make_ndx and distance		08/04/2017 12:24 PM	
2224	GROMACS	Feature	New	Normal	Proposed feature: conditional stop	Vedran Miletic	09/19/2018 03:06 PM	2020

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