

Issues

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
3205	GROMACS	Task	New	High	address Debian experimental issues		11/18/2019 11:17 AM	2020-beta3
3189	GROMACS	Task	New	High	implement heuristics for switching between different spread/gather kernel layouts	Jonathan Vincent	11/16/2019 08:50 PM	2020-beta3
3163	GROMACS	Bug	New	High	gpuupdate / task assignment stabilization	Artem Zhmurov	11/14/2019 06:01 PM	2020-beta3
3125	GROMACS	Bug	New	Normal	OpenCL on Volta and Turing borken		11/04/2019 11:37 AM	2020-beta3
3195	GROMACS	Task	New	High	assess nightly master failures		11/01/2019 09:21 PM	2020-beta3
2958	GROMACS	Bug	New	Normal	Compiling master (to become 2020) using CUDA 9.0		11/01/2019 03:24 PM	2020-beta3
2990	GROMACS	Bug	New	Normal	ARM neon SIMD4 error		11/01/2019 03:24 PM	2020-beta3
3017	GROMACS	Bug	New	Normal	ddBalanceRegionHandler triggers need fixing		11/01/2019 03:23 PM	2020-beta3
3097	GROMACS	Bug	New	Normal	nbnxm grid issue with regressiontest complex/nbnxn_rzero with gpubufferops path		11/01/2019 03:22 PM	2020-beta3
3193	GROMACS	Bug	New	Normal	Unused parameter warnings in pme code	Paul Bauer	11/01/2019 09:40 AM	2020-beta3
2967	GROMACS	Feature	New	Normal	GPU reallocateDeviceBuffer improvements		10/31/2019 03:35 PM	2020-beta3
3136	GROMACS	Bug	New	Normal	gmxapi.operation data flow topology unclear or incomplete	Eric Irrgang	10/22/2019 03:09 PM	2020-beta3
3130	GROMACS	Task	New	Normal	Interim handling of gmxapi data references.	Eric Irrgang	10/22/2019 03:09 PM	2020-beta3
3167	GROMACS	Task	New	Normal	GPU update path user documentation		10/21/2019 04:09 PM	2020-beta3
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
2722	GROMACS	Bug	New	Normal	gmxapi may over-manage RPATH	Mark Abraham	10/16/2019 10:28 AM	2020-beta3
3200	GROMACS	Bug	Accepted	Normal	Segmentation Fault in gmx mdrun in gromacs 2020-beta1 and hwloc 2.0.2	Paul Bauer	11/17/2019 11:10 PM	2020-beta3
2737	GROMACS	Bug	Accepted	Low	AMD OpenCl failies release build in complex tests	Szilárd Páll	11/01/2019 03:25 PM	2020-beta3
3183	GROMACS	Task	Accepted	Normal	enable bonded interactions on GPU		10/31/2019 11:49 AM	2020-beta3
3164	GROMACS	Bug	In Progress	High	mdrun-mpi-test with separate PME ranks and PP-PME CPU comm crashes	Alan Gray	11/14/2019 12:41 PM	2020-beta3
3160	GROMACS	Feature	In Progress	High	implement direct comm for different src/target memory spaces	Alan Gray	11/11/2019 04:43 PM	2020-beta3
3093	GROMACS	Task	In Progress	High	rework GPU direct halo-exchange related force reduction complexities		11/01/2019 08:58 PM	2020-beta3
2817	GROMACS	Feature	In Progress	High	GPU X/F buffer ops		11/01/2019 04:28 PM	2020-beta3
3029	GROMACS	Feature	In Progress	High	GPU force buffer ops + reduction		11/01/2019 04:28 PM	2020-beta3
3142	GROMACS	Feature	In Progress	High	centralize and clarify GPU force buffer clearing		11/01/2019 04:28 PM	2020-beta3
3027	GROMACS	Task	In Progress	Normal	Move sample_restraint development from GitHub to Gerrit	Eric Irrgang	11/01/2019 03:23 PM	2020-beta3
3159	GROMACS	Task	In Progress	High	eliminate regression due to moving gmx_pme_send_coordinates()	Alan Gray	11/01/2019 11:26 AM	2020-beta3
2998	GROMACS	Task	In Progress	Normal	Update Python detection		10/29/2019 05:42 PM	2020-beta3

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2756	GROMACS	Task	In Progress	Normal	gmxapi integration testing		10/29/2019 05:38 PM	2020-beta3
3175	GROMACS	Task	Fix uploaded	Normal	update bundled pybind11 headers to v2.4.3 for Python 3.8 updates	Eric Irrgang	10/25/2019 11:28 AM	2020-beta3
3168	GROMACS	Feature	New	Normal	GPU update release notes		11/14/2019 06:03 PM	2020-rc1
3131	GROMACS	Task	New	Normal	support ccache with clang-tidy	Mark Abraham	10/29/2019 05:41 PM	2020-rc1
2979	GROMACS	Task	Accepted	Normal	Reconsider default 1 OpenMP thread per thread-MPI rank	Berk Hess	11/01/2019 03:24 PM	2020-rc1
3010	GROMACS	Task	In Progress	Normal	upgrade OpenCL stack on bs-gpu01		10/29/2019 05:41 PM	2020-rc1
3206	GROMACS	Bug	New	Normal	2 not-critical bugs in analyse tool		11/15/2019 03:53 PM	2019.5
2974	GROMACS	Bug	New	Normal	position-restraints regressiontest fails on intel GPU		10/01/2019 11:12 AM	2019.5
3178	GROMACS	Bug	Accepted	Normal	Fatal Error when launching mdrun on host with busy/unavailable GPU(s)	Szilárd Páll	10/28/2019 10:38 PM	2019.5
3204	GROMACS	Bug	Fix uploaded	Normal	intermolecular interactions on OpenMPI multiple threads (gromacs 2019.4)	Berk Hess	11/18/2019 04:42 PM	2019.5
3203	GROMACS	Bug	Fix uploaded	Normal	Segmentation fault using gmx solvent	Paul Bauer	11/16/2019 06:27 PM	2019.5
3173	GROMACS	Bug	Resolved	Normal	Illegal memory access in free-energy calculations	Berk Hess	10/23/2019 01:30 PM	2019.5
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
2927	GROMACS	Bug	Feedback wanted	Low	CMake 3.14.1 fails to properly run gmxDetectCpu.make		11/12/2019 10:30 AM	2019.5
3208	GROMACS	Task	New	High	improve PP-PME tuning		11/18/2019 09:39 PM	2020
3124	GROMACS	Bug	New	Normal	significant performance loss due to DLB auto-off when PP/PME load >1		11/18/2019 09:37 PM	2020
1826	GROMACS	Task	New	Normal	investigate non-optimal results with CPU-GPU balancing on AMD	Szilárd Páll	11/18/2019 09:35 PM	2020
2985	GROMACS	Feature	New	Normal	Python package documentation		11/08/2019 08:55 PM	2020
3188	GROMACS	Task	New	Normal	re-enable parallel spline calculation for #threads/atoms > 4		11/03/2019 09:18 PM	2020
2816	GROMACS	Feature	New	High	GPU offload / optimization for update&constraints, buffer ops and multi-gpu communication	Alan Gray	11/01/2019 06:56 PM	2020
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
2987	GROMACS	Bug	New	Normal	assess the bonded GPU task assignment default		10/21/2019 04:15 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
2888	GROMACS	Feature	New	High	CUDA Update and Constraints module	Artem Zhmurov	10/21/2019 03:59 PM	2020
3161	GROMACS	Bug	New	Normal	mdrun-test hangs with -ntmpi2		10/17/2019 05:34 PM	2020
2890	GROMACS	Feature	New	High	GPU Halo Exchange		10/17/2019 02:00 PM	2020
3141	GROMACS	Bug	New	Normal	gmxapi File placeholders missing from beta release	Eric Irrgang	10/15/2019 03:57 PM	2020

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3140	GROMACS	Feature	New	Normal	Allow explicit input definition for gmxapi.operation function wrapper	Eric Irrgang	10/15/2019 03:56 PM	2020
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
3133	GROMACS	Task	New	Normal	Cookiecutter for sample_restraint	Eric Irrgang	10/13/2019 01:07 PM	2020
3082	GROMACS	Task	New	High	move launch/synchronization points to clarify task dependencies		10/11/2019 05:53 PM	2020
3119	GROMACS	Task	New	Normal	clang-tidy coverage of parallelization codepaths		10/04/2019 12:17 PM	2020
2886	GROMACS	Feature	New	Normal	CUDA version of SETTLE	Artem Zhmurov	10/02/2019 12:02 PM	2020
2887	GROMACS	Feature	New	Normal	CUDA version of Leap Frog algorithm	Artem Zhmurov	10/02/2019 12:00 PM	2020
2934	GROMACS	Feature	New	Normal	GPU X Buffer ops		09/24/2019 06:07 PM	2020
3037	GROMACS	Task	New	Normal	add missing cycle counters related to buffer ops/reduction launches		09/24/2019 03:27 PM	2020
2992	GROMACS	Task	New	Normal	Split hw_opt in const user options and dynamic settings		09/24/2019 03:23 PM	2020
3104	GROMACS	Task	New	Normal	implement GPU DD cycle counting		09/24/2019 03:19 PM	2020
3105	GROMACS	Task	New	Normal	implement GPU PME/PP comm cycle counting		09/24/2019 03:19 PM	2020
3092	GROMACS	Task	New	Normal	implement better receiver ready / notify in halo exchange		09/18/2019 02:47 AM	2020
2053	GROMACS	Task	New	Normal	refine notation in GPU code		09/04/2019 01:47 PM	2020
3064	GROMACS	Task	New	Normal	add test for perturbed bonded forces		08/22/2019 06:34 PM	2020
3031	GROMACS	Task	New	Normal	evaluate the impact of particle order on PME		08/21/2019 06:08 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
2976	GROMACS	Task	New	Normal	Basic math for Multidimensional arrays		08/04/2019 09:44 PM	2020
3026	GROMACS	Task	New	Normal	add flags for GPU force buffer op / reduction activation		08/01/2019 04:46 PM	2020
3050	GROMACS	Bug	New	Low	Fix tests on Solaris	Vedran Miletic	07/29/2019 12:38 PM	2020
3038	GROMACS	Feature	New	Normal	Improvements to MD plugin development environment	Eric Irrgang	07/17/2019 02:15 PM	2020
3032	GROMACS	Feature	New	Normal	Clean up dev-manual structure		07/11/2019 11:48 AM	2020
3024	GROMACS	Bug	New	Normal	Bad logic for Sphinx detection CMake output		07/05/2019 05:44 PM	2020
3014	GROMACS	Task	New	Normal	gmxapi example Python scripts		06/28/2019 11:07 AM	2020
3008	GROMACS	Task	New	Normal	verify block size choice of CUDA bonded kernel		06/26/2019 08:38 PM	2020
3001	GROMACS	Task	New	Normal	explore simplifying virial and shift force reduction		06/25/2019 04:03 PM	2020
2997	GROMACS	Task	New	Normal	improve performance of alchemical free energy calculations		06/24/2019 03:07 PM	2020
2996	GROMACS	Feature	New	Normal	gmxapi execution model	Eric Irrgang	06/24/2019 02:16 PM	2020
2994	GROMACS	Feature	New	Normal	Data flow topology in gmxapi 2020		06/24/2019 01:53 PM	2020
2965	GROMACS	Task	New	Normal	Performance of GPU direct communications		05/31/2019 03:12 PM	2020
2943	GROMACS	Task	New	Normal	Rename Integrator	Pascal Merz	05/23/2019 08:04 PM	2020

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2957	GROMACS	Feature	New	Normal	add support for the Hygon Dhyana architecture		05/21/2019 01:00 PM	2020
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
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
2944	GROMACS	Feature	New	Normal	Roadmap for thermostats / barostats in new propagation/integration scheme	Michael Shirts	05/08/2019 05:50 PM	2020
2925	GROMACS	Bug	New	Normal	BasicVector addition operator yields unexpected result when adding scalar	Christian Blau	04/20/2019 05:39 PM	2020
2839	GROMACS	Task	New	Normal	make module and file naming consistent		04/09/2019 04:27 PM	2020
2699	GROMACS	Task	New	Normal	Test POWER9		04/05/2019 04:50 PM	2020
2877	GROMACS	Task	New	Normal	use gm::Options more	Mark Abraham	04/02/2019 06:14 PM	2020
2833	GROMACS	Task	New	Normal	Update topology datastructures	Paul Bauer	04/02/2019 12:39 PM	2020
2774	GROMACS	Feature	New	Normal	Refactor shell code into its own integrator	David van der Spoel	03/29/2019 05:20 PM	2020
2901	GROMACS	Feature	New	Normal	Declare external Resources in mdp / tpr files.	Christian Blau	03/27/2019 04:27 PM	2020
2885	GROMACS	Feature	New	Normal	CUDA version of LINCS	Artem Zhmurov	03/12/2019 01:33 PM	2020
2889	GROMACS	Task	New	Normal	update grompp warnings for brevity, usefulness and actionability	Mark Abraham	03/11/2019 02:15 PM	2020
2795	GROMACS	Task	New	Normal	Incorporate regressiontests into core gromacs		02/13/2019 08:17 PM	2020
2832	GROMACS	Bug	New	Low	PaddedVector move operations broken	Mark Abraham	02/12/2019 03:22 PM	2020
2834	GROMACS	Task	New	Normal	C++ matrix classes	Christian Blau	01/23/2019 12:19 PM	2020
2695	GROMACS	Task	New	Low	bonded GPU module timing		01/21/2019 01:19 PM	2020
1587	GROMACS	Task	New	Normal	improve the configurability of regression tests		01/18/2019 06:17 AM	2020
2518	GROMACS	Task	New	Normal	redesign task-assignment code for OpenCL		12/28/2018 12:38 PM	2020
2480	GROMACS	Bug	New	Normal	pdb2gmx does not protonate correctly for united-atom Gromos	Mark Abraham	12/17/2018 01:27 PM	2020
2806	GROMACS	Feature	New	Normal	SIMD algorithms for ARM SVE // nobbonded 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
2697	GROMACS	Task	New	Normal	improve FFT library flavor/version reporting		12/10/2018 01:49 PM	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
2425	GROMACS	Task	New	Normal	testing multisim with multiple ranks per simulation	Mark Abraham	11/29/2018 11:20 AM	2020
2686	GROMACS	Task	New	Normal	add tests for gpu bonded interactions		11/29/2018 10:44 AM	2020
2773	GROMACS	Task	New	Normal	improve GPU error handling and make such handling uniform across modules		11/21/2018 10:28 AM	2020
2767	GROMACS	Bug	New	Normal	grompp warns about md + FEP even for fully coupled states		11/19/2018 11:41 AM	2020

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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
2715	GROMACS	Feature	New	Normal	Avoid requesting the user to recompile gromacs for Intel OpenCL support		10/31/2018 12:16 PM	2020
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
2537	GROMACS	Task	New	Normal	Simplify PME solve reduction	Aleksei lupinov	10/30/2018 12:08 PM	2020
2498	GROMACS	Task	New	Normal	OpenCL memory pinning/mapping		10/30/2018 12:07 PM	2020
2522	GROMACS	Task	New	Normal	OpenCL context duplication		10/30/2018 12:07 PM	2020
2524	GROMACS	Task	New	Normal	struct alignment/packing for OpenCL host & device code		10/30/2018 12:06 PM	2020
2475	GROMACS	Task	New	Normal	make OpenCL 1st class-citizen in the build system		10/30/2018 12:01 PM	2020
2353	GROMACS	Task	New	Normal	improve on relative tolerance for constructing tables		10/30/2018 04:17 AM	2020
2710	GROMACS	Feature	New	Normal	Separate dvdI for each molecule (of couple-moltype) when running FEP		10/26/2018 10:24 AM	2020
2169	GROMACS	Task	New	Normal	remove 'continuation' mdp option		10/12/2018 10:36 PM	2020
2495	GROMACS	Task	New	Normal	replace -noconfout with mdp option	Mark Abraham	10/12/2018 10:34 PM	2020
2396	GROMACS	Task	New	Normal	Refactor trajectoryanalysis module to allow handling of trajectory frame manipulation	Paul Bauer	10/08/2018 07:29 PM	2020
2671	GROMACS	Task	New	Normal	replace constants like M_PI		10/05/2018 08:58 AM	2020
2481	GROMACS	Task	New	Low	Update gmx report-methods to write more method information		09/20/2018 07:43 AM	2020
2224	GROMACS	Feature	New	Normal	Proposed feature: conditional stop	Vedran Miletic	09/19/2018 03:06 PM	2020
2054	GROMACS	Feature	Accepted	High	PME on GPU	Aleksei lupinov	10/03/2019 09:41 PM	2020
3071	GROMACS	Bug	Accepted	Normal	complex.nbxn-ljpme-LB-geometric failing with OpenCL timing debug mode assertions	Szilárd Páll	09/02/2019 10:19 PM	2020
2875	GROMACS	Task	Accepted	Normal	SIMD version of the free-energy kernel	Berk Hess	08/26/2019 03:47 PM	2020
2615	GROMACS	Feature	Accepted	Normal	Switch to Python3		07/05/2019 02:57 PM	2020
1165	GROMACS	Feature	Accepted	Low	Multi-SIMD binaries		01/23/2019 02:08 PM	2020
2391	GROMACS	Task	Accepted	Normal	re-enable TPI test	Berk Hess	01/09/2019 05:17 PM	2020
2822	GROMACS	Task	Accepted	Normal	Make nbxn a module	Berk Hess	01/03/2019 03:07 PM	2020
1943	GROMACS	Task	Accepted	Low	make sure releases are submitted early for Debian Experimental	Szilárd Páll	12/31/2018 11:15 AM	2020
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

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2553	GROMACS	Bug	Accepted	Normal	Incorrect COM velocity correction with frozen atoms	Berk Hess	12/03/2018 01:15 PM	2020
2706	GROMACS	Task	Accepted	Normal	Rework classic QM/MM interface		11/05/2018 10:06 AM	2020
2581	GROMACS	Feature	Accepted	Normal	User interface for hybrid Monte Carlo		10/15/2018 05:21 PM	2020
1781	GROMACS	Task	Accepted	Normal	re-design benchmarking functionality	Mark Abraham	10/08/2018 07:04 PM	2020
2675	GROMACS	Task	In Progress	Normal	bonded CUDA offload task		10/29/2019 03:11 PM	2020
2896	GROMACS	Feature	In Progress	Normal	Python packaging		10/09/2019 04:08 PM	2020
2281	GROMACS	Task	In Progress	Normal	Represent data on regularly spaced N-dimensional grids.	Christian Blau	08/06/2019 08:48 AM	2020
1925	GROMACS	Task	In Progress	Normal	remove concept of unilateral global communication		07/15/2019 06:42 PM	2020
2988	GROMACS	Task	In Progress	Low	clean up and refactor code to modern standards		06/20/2019 02:14 PM	2020
2862	GROMACS	Bug	In Progress	Normal	Division by zero in restrained dihedrals		04/01/2019 11:53 AM	2020
868	GROMACS	Feature	In Progress	Normal	Implement parallelization support to analysis framework	Kevin Boyd	02/07/2019 02:08 AM	2020
2727	GROMACS	Task	In Progress	Low	Move non-analysis functions out of gmxana		01/20/2019 07:48 PM	2020
2766	GROMACS	Task	In Progress	Normal	Improve hardware option selection	Kevin Boyd	12/20/2018 06:40 PM	2020
2059	GROMACS	Task	In Progress	Normal	Separate different types of data in t_state		10/12/2018 10:36 PM	2020
2070	GROMACS	Feature	In Progress	Normal	Physical validation testing	Michael Shirts	10/12/2018 10:36 PM	2020
2395	GROMACS	Task	In Progress	Normal	break up commrec	Mark Abraham	09/19/2018 03:13 PM	2020
1985	GROMACS	Bug	Fix uploaded	Low	CUDA build system refactoring awaiting review		10/15/2018 05:21 PM	2020
3022	GROMACS	Feature	Resolved	Normal	modernized naming for new GPU developments		11/11/2019 01:03 PM	2020
2893	GROMACS	Task	Resolved	Normal	Integrate gmxapi Python package	Eric Irrgang	10/23/2019 09:16 AM	2020
2453	GROMACS	Task	Resolved	High	PME OpenCL porting effort	Aleksei lupinov	06/05/2019 05:32 PM	2020
2894	GROMACS	Task	Resolved	Normal	Wrap importable Python code.	Eric Irrgang	05/09/2019 11:30 AM	2020
2895	GROMACS	Task	Resolved	Normal	gmxapi Output proxy establishes execution dependency.	Eric Irrgang	03/29/2019 05:18 PM	2020
3021	GROMACS	Feature	Feedback wanted	Normal	Completion of docs for GPU developments		11/01/2019 06:29 PM	2020
2390	GROMACS	Bug	Feedback wanted	Normal	GROMACS build system should check for valid nvcc flags before use		01/30/2019 06:16 PM	2020
1977	GROMACS	Bug	Feedback wanted	Low	warning: __WORDSIZE not defined		09/21/2018 06:19 PM	2020
3197	GROMACS	Bug	New	Normal	Rework usage of gitattributes and filter in source code formatting scripts		11/04/2019 12:50 PM	2021-infrastructure-stable
3150	GROMACS	Bug	New	Normal	gmxapi data type annotations are confusing and inadequate	Eric Irrgang	10/22/2019 03:08 PM	2021-infrastructure-stable
3152	GROMACS	Feature	New	Low	Infrastructure and patterns for expressing public interfaces		10/17/2019 10:40 AM	2021-infrastructure-stable
3153	GROMACS	Task	New	Low	Let CMake process module directories earlier to support more modern CMake idioms.		10/17/2019 10:40 AM	2021-infrastructure-stable
3148	GROMACS	Feature	New	Normal	Roadmap for gmxapi filesystem interactions.	Eric Irrgang	10/15/2019 06:23 PM	2021-infrastructure-stable

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3147	GROMACS	Feature	New	Normal	gmxapi workflow checkpointing	Eric Irrgang	10/15/2019 06:18 PM	2021-infrastructure-stable
3113	GROMACS	Bug	New	Low	Use of read_tps_conf is depeccrated	Paul Bauer	10/01/2019 11:36 AM	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
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
2916	GROMACS	Task	New	Normal	Decide future of symtab	Paul Bauer	09/06/2019 02:35 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
3035	GROMACS	Task	New	Normal	Provide central logger in wrapper binary	Paul Bauer	09/06/2019 02:34 PM	2021-infrastructure-stable
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
3072	GROMACS	Task	New	Normal	Use gmx::index for indexing instead of int	Christian Blau	09/03/2019 04:23 PM	2021-infrastructure-stable
3047	GROMACS	Task	New	Normal	Set required versions for GROMACS 2021		08/24/2019 05:25 PM	2021-infrastructure-stable
3155	GROMACS	Task	Accepted	Normal	Unify DD and CPU-GPU gather & scatter	Artem Zhmurov	10/17/2019 03:50 PM	2021-infrastructure-stable
3033	GROMACS	Task	In Progress	Normal	Clean up and modernize googletest bundling and usage		08/24/2019 05:23 PM	2021-infrastructure-stable
3207	GROMACS	Task	New	Normal	Ad cycle counting to StatePropagatorDataGpu		11/18/2019 06:04 PM	
3114	GROMACS	Task	New	Low	Possible improvements to update-constraints	Artem Zhmurov	11/14/2019 06:06 PM	
3180	GROMACS	Task	New	Normal	Remove extra D2H and H2D copies of coordinates when the COM motion is compensated.	Artem Zhmurov	11/14/2019 05:48 PM	
3202	GROMACS	Bug	New	Low	gmx solvate fails to overwrite topology file		11/13/2019 02:44 PM	
3177	GROMACS	Feature	New	Normal	Spack package management support		11/06/2019 06:37 PM	
3198	GROMACS	Bug	New	Normal	Fails to build on FreeBSD with Clang since f7940fa01e8b6ef0703236b53721cca2d81b40d3 Use gmock and gtest targets from googletest-release-1.8.0		11/06/2019 12:20 PM	
3196	GROMACS	Bug	New	Normal	ExponentialMovingAverage.DeterminesCorrectlyIfIncreasing failing		11/01/2019 11:28 PM	
3194	GROMACS	Task	New	Normal	consider passing GPU dependency list to both dependency producers and consumers		11/01/2019 07:10 PM	
2891	GROMACS	Feature	New	High	PME/PP GPU communications		11/01/2019 06:56 PM	
3132	GROMACS	Task	New	Normal	gmxapi testing support tools		10/31/2019 03:35 PM	
2792	GROMACS	Task	New	High	Improvement of PME gather and spread CUDA kernels		10/30/2019 01:29 PM	
3187	GROMACS	Task	New	Normal	Template updated PME kernels using threads per atom		10/30/2019 11:33 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	
2126	GROMACS	Feature	New	Normal	implement native CUDA support in CMake		10/29/2019 09:03 PM	
3182	GROMACS	Bug	New	Normal	pressure coupling buggy with GPU update		10/28/2019 11:34 PM	

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
3181	GROMACS	Task	New	Normal	consolidate task assignment and workload data initialization		10/28/2019 02:53 PM	
3179	GROMACS	Feature	New	Normal	Clarify access to parallel data outputs	Eric Irrgang	10/26/2019 12:23 PM	
2915	GROMACS	Feature	New	High	GPU direct communications		10/24/2019 10:59 AM	
2045	GROMACS	Task	New	Normal	API design and language bindings	Peter Kasson	10/23/2019 09:16 AM	
3162	GROMACS	Feature	New	Normal	Add virtual site support to GPU version of update-constraints.		10/21/2019 03:59 PM	
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	
3157	GROMACS	Task	New	Normal	separate PME x receive sync	Alan Gray	10/17/2019 02:44 PM	
3154	GROMACS	Task	New	Low	Update use of Python subprocess for >=3.5		10/17/2019 01:46 PM	
2993	GROMACS	Feature	New	Normal	Scalar and structured type expression and definitions for API	Eric Irrgang	10/17/2019 09:55 AM	
3149	GROMACS	Feature	New	Normal	Python user interface for obtaining simulation artifacts as files.	Eric Irrgang	10/15/2019 06:21 PM	
3138	GROMACS	Feature	New	Normal	Improve ensemble support in Context specification.		10/15/2019 03:56 PM	
3139	GROMACS	Task	New	Normal	gmxapi Futures should be subscribable	Eric Irrgang	10/15/2019 03:56 PM	
3135	GROMACS	Feature	New	Normal	Make GPU traits ino opaque types		10/14/2019 10:24 AM	
3042	GROMACS	Bug	New	Normal	core dump error in grompp command		10/09/2019 07:30 PM	
3127	GROMACS	Bug	New	Normal	mdrun-mpi-test -ntmpi 2 runs out of memory with OpenCL on Nvidia		10/09/2019 05:33 PM	
3126	GROMACS	Feature	New	Normal	State propagator GPU data manager		10/09/2019 02:42 PM	
3123	GROMACS	Task	New	Normal	address sanitizer coverage of parallelization code-paths		10/05/2019 12:32 AM	
3116	GROMACS	Bug	New	Normal	regressiontests/freenenergy 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	
2961	GROMACS	Feature	New	Normal	How should Python package find GROMACS resources under various circumstances?		10/02/2019 02:06 PM	
3086	GROMACS	Bug	New	Normal	gmxapi fails with MPI build of GROMACS 2020		09/25/2019 04:18 PM	
3088	GROMACS	Bug	New	Normal	Reference to theory needed for cylindrical pull geometry		09/13/2019 11:26 AM	
3083	GROMACS	Bug	New	Normal	Listed forces tests failing on ICC19 with AVX2_256 nightly build		09/10/2019 11:56 AM	
3078	GROMACS	Task	New	Normal	Allow MD modules to register energy output fields themselves		09/06/2019 11:36 AM	
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	
687	Support Platforms	Feature	New	Normal	Add content on the front page		09/02/2019 01:08 PM	
1500	GROMACS	Feature	New	Normal	Post-5.0 feature clean-up plan	Mark Abraham	08/26/2019 03:47 PM	
3068	GROMACS	Bug	New	Normal	Misleading warning on rerun		08/26/2019 03:44 PM	

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
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	
2905	GROMACS	Task	New	Normal	Add a Jenkins configuration with std library assert		08/24/2019 05:22 PM	
3020	GROMACS	Feature	New	Low	modernize DeviceBuffer and GPU memory management		08/13/2019 06:01 PM	
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	
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	
3041	GROMACS	Task	New	Normal	Remove workaround for gcc bug 58265		07/23/2019 12:27 PM	
3045	GROMACS	Feature	New	Low	Option to remove v-sites in trjconv?		07/19/2019 04:42 PM	
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	
2907	GROMACS	Bug	New	Normal	Gromacs autocompletion appears to be broken with ZSH		07/16/2019 04:46 AM	
2983	GROMACS	Task	New	Normal	better suited data-types for bonded GPU kernels		07/11/2019 04:32 PM	
3030	GROMACS	Feature	New	Normal	RST style guidelines		07/09/2019 03:38 PM	
2949	GROMACS	Bug	New	Normal	cmake fails when building mdrun only		07/08/2019 10:04 AM	
3005	GROMACS	Task	New	Normal	Move logging in gmx 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	
3000	GROMACS	Bug	New	Normal	CMake "webpage" target does not fail when it should		06/25/2019 02:43 PM	
2984	GROMACS	Feature	New	Normal	More Extensive Selections Examples	Dallas Warren	06/18/2019 11:50 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	
2975	GROMACS	Feature	New	Normal	LJ PME calculations on GPUs		06/12/2019 01:17 PM	
2516	GROMACS	Task	New	Low	Support PME OpenCL execution width < 16	Aleksei lupinov	06/05/2019 05:32 PM	
2954	GROMACS	Bug	New	Normal	genion changes residue numbering		05/26/2019 12:08 AM	
2948	GROMACS	Bug	New	Normal	SIMD support detected as none on AMD R5 2500U		05/21/2019 12:58 PM	
2956	GROMACS	Feature	New	Normal	SAXS resolution		05/17/2019 09:58 AM	
2596	GROMACS	Feature	New	Normal	Constant potential method	Benson Muite	05/10/2019 09:54 AM	

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
2570	GROMACS	Feature	New	Normal	Better string formatting and printing		05/02/2019 12:20 PM	
2375	GROMACS	Task	New	Normal	Clarify execution phases for MD simulation		04/30/2019 12:59 PM	
2902	GROMACS	Bug	New	Normal	2019.1 equilibration issue? (Intel 2018u3)		04/30/2019 08:17 AM	
2931	GROMACS	Feature	New	Normal	Tables in Verlet kernels		04/29/2019 12:01 PM	
2937	TNG trajectory library	Bug	New	Normal	tng_num_frames_get reports incorrect num frames		04/29/2019 11:30 AM	
2930	GROMACS	Feature	New	Normal	Limited range for reference group detection in cylinder pulling		04/26/2019 05:17 PM	
2933	GROMACS	Task	New	Normal	Convert walls to a ForceProvider		04/25/2019 02:43 PM	
2928	GROMACS	Feature	New	Normal	Add ability to use expression "count of ATOM_EXPR" in selection statements.		04/16/2019 04:52 PM	
2919	GROMACS	Task	New	Normal	C++ style guidelines for namespace use		04/15/2019 01:21 PM	
2924	GROMACS	Bug	New	Normal	Failing version check when reading new tpr file with older gromacs version		04/12/2019 10:52 AM	
2910	GROMACS	Feature	New	Normal	Mixed scaling for 1-4 interactions		04/10/2019 10:13 PM	
2897	GROMACS	Bug	New	Normal	rotation/flex2 can still fail on cpu-only run on OpenCL build		04/04/2019 06:24 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	
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	
2876	GROMACS	Bug	New	Normal	2019.1 make check fails on AVX and AVX2 (Intel 2018u3)	Erik Lindahl	03/08/2019 10:32 AM	
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	
2869	GROMACS	Bug	New	Normal	GPU detection error only issued as a note to the log		03/05/2019 04:09 PM	
2870	GROMACS	Bug	New	Normal	GPU detection error message missing from the output		03/05/2019 03:55 PM	
2698	GROMACS	Task	New	Normal	gmxapi documentation integration		03/02/2019 01:31 AM	
2873	GROMACS	Bug	New	Normal	Simple way to get last frame from trajectory		02/28/2019 11:14 PM	
2874	GROMACS	Task	New	Normal	Refactor Gromacs (cluster) neighborlist into separate module	Erik Lindahl	02/28/2019 11:36 AM	
2872	GROMACS	Bug	New	Normal	gmx solvate and genion topology update		02/27/2019 10:18 AM	
2755	GROMACS	Feature	New	Low	md5 sums and sha256, sha512 hashes	Benson Muite	02/19/2019 11:00 PM	
2864	GROMACS	Task	New	Normal	Building incompatibilities	Benson Muite	02/19/2019 02:00 PM	
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	
2860	GROMACS	Feature	New	Normal	Option for outputting min/max coordinates in gmx traj		02/08/2019 12:35 AM	

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
2835	GROMACS	Task	New	Normal	Matrix class constraint to upper or lower triangle		02/07/2019 02:44 PM	
2754	GROMACS	Bug	New	Normal	Simulated Tempering seems to be broken	Michael Shirts	02/05/2019 03:58 PM	
2853	GROMACS	Bug	New	Normal	EwaldUnitTests segfault on armv7hl with gcc-9.0.1	Paul Bauer	02/04/2019 05:34 PM	
2854	GROMACS	Bug	New	Normal	OnlineHelpUnitTests segfaults on s390x with gcc-9.0.1	Paul Bauer	02/04/2019 11:17 AM	
2248	GROMACS	Feature	New	Normal	Label all SIMD functions as pure/nodiscard		02/04/2019 04:49 AM	
2857	GROMACS	Task	New	Normal	Clarify recommended function specifies (constexpr, noexcept, pure)		02/04/2019 04:48 AM	
2846	GROMACS	Feature	New	Low	Set rpath in FindLibStdCpp.cmake		02/02/2019 08:09 AM	
2855	GROMACS	Task	New	Normal	Allow compiling GROMACS without C compiler		01/31/2019 08:44 PM	
2852	GROMACS	Bug	New	Low	the in-tree regressiontest download can get out of sync with code		01/30/2019 03:58 PM	
2851	Support Platforms	Task	New	Normal	uninstall redmine checklist plugin		01/30/2019 03:33 PM	
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	
1354	GROMACS	Bug	New	Normal	Constant acceleration NEMD is broken.	David van der Spoel	01/09/2019 04:42 PM	
2239	GROMACS	Feature	New	Normal	split libgromacs into base and full		01/07/2019 01:47 AM	
2788	GROMACS	Bug	New	Normal	PME will not run on AMD GPU with NVidia GPU present		01/03/2019 02:24 PM	
2796	GROMACS	Task	New	Low	clarify what mdrun -cpt means		01/03/2019 02:09 PM	
1505	GROMACS	Task	New	Normal	improve handling of logging	Mark Abraham	01/02/2019 06:06 PM	
1323	GROMACS	Task	New	Normal	determine future of existing tools for	David van der Spoel	12/04/2018 11:53 AM	
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	
2764	GROMACS	Task	New	Normal	gmxapi version updates for post release-2019	Eric Irrgang	11/21/2018 12:53 PM	
2761	GROMACS	Feature	New	Low	lincs-order 4 is too conservative for some force fields		11/16/2018 09:55 AM	
2739	GROMACS	Feature	New	Normal	Parallel continuous tempering and enhanced sampling feature		11/13/2018 11:36 PM	
2065	GROMACS	Bug	New	Normal	thread-MPI internal errors		11/08/2018 03:43 PM	
2740	GROMACS	Bug	New	Normal	mdrun reports incorrect error with -bonded gpu without gpu	Mark Abraham	11/07/2018 01:59 PM	
2707	GROMACS	Bug	New	Normal	Installed OpenCL files include clh file from gpu_utils directory		10/30/2018 04:02 AM	
2713	GROMACS	Feature	New	Normal	Constant offset for external electric fields		10/28/2018 12:57 AM	
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	

#	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	
2645	GROMACS	Bug	New	Normal	Security		09/28/2018 01:16 PM	
2657	GROMACS	Bug	New	Normal	Biphasic tutorial		09/28/2018 10:02 AM	
2608	GROMACS	Task	New	Normal	Remove code duplication between OpenCL and CUDA		09/24/2018 12:47 PM	
2616	GROMACS	Task	New	Normal	Model for MD state		09/14/2018 05:12 PM	
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	
2624	GROMACS	Bug	New	Normal	GPU build system not robust enough		09/05/2018 02:00 AM	
2611	GROMACS	Bug	New	Normal	issues with gpu_utils-test with GMX_BUILD_UNITTESTS=OFF and on OSX		08/14/2018 07:03 PM	
2602	GROMACS	Bug	New	Low	build information gets outdated if build tree is reused		08/13/2018 09:04 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	
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	
2531	GROMACS	Task	New	Low	Consider optimizing tabulated data access on GPU		07/30/2018 12:31 PM	
2576	GROMACS	Bug	New	Normal	gmx potential -correct outputs the wrong potential		07/25/2018 02:58 PM	
2573	GROMACS	Bug	New	High	Different mdp files describing the same change yield different free energy on the same trajectory		07/19/2018 06:52 PM	
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	
2555	GROMACS	Bug	New	Low	building GROMACS 2018.2		07/03/2018 11:41 PM	
2563	GROMACS	Bug	New	Normal	Windows 7 Compilation with GPU support		07/02/2018 09:58 AM	
2010	GROMACS	Task	New	Normal	Use size_t instead of int for indexing		07/01/2018 07:57 AM	
2556	GROMACS	Feature	New	Normal	make default selections suitable for DNA and RNA	Mark Abraham	06/20/2018 01:48 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	
2538	GROMACS	Task	New	Normal	organize more of the PME GPU code along task-specific lines	Mark Abraham	05/31/2018 05:41 PM	
2535	GROMACS	Task	New	Normal	consider compiling opencl fft kernels once		05/31/2018 01:33 PM	
2526	GROMACS	Bug	New	Normal	Bug of gmx hbond		05/30/2018 03:12 PM	

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
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	
2473	GROMACS	Bug	New	Normal	mdrun sometimes stalls due to large coordinates with no constraints		04/04/2018 10:15 PM	
2460	GROMACS	Bug	New	Normal	Allow inclusion of user libraries through CMake cache variables		03/28/2018 08:47 PM	
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	
2462	GROMACS	Task	New	Normal	consider adding STL misuse tests		03/23/2018 01:23 AM	
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	
2429	GROMACS	Feature	New	Normal	Add option of periodic chain topology to pdb2gmx		03/10/2018 01:01 PM	
2113	GROMACS	Bug	New	Normal	Google tests and execution order		03/05/2018 02:05 PM	
2435	GROMACS	Task	New	Normal	identify and note about/tune task offload in GPU-bound runs		03/02/2018 04:08 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	
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	
2393	GROMACS	Bug	New	Normal	incorrect error message with omitted command line flag before its argument		01/24/2018 11:24 PM	
1842	GROMACS	Feature	New	Normal	Replace XML with JSON		01/18/2018 05:12 PM	
2380	GROMACS	Bug	New	Low	cycle counter issues with separate PME rank + GPUs		01/16/2018 10:21 PM	
2382	GROMACS	Task	New	Normal	Simplify Doxygen guidelines		01/13/2018 12:40 AM	
2231	GROMACS	Bug	New	Normal	convert-tpv aborts when saving subset of the system		01/12/2018 03:52 PM	
2052	GROMACS	Bug	New	Low	trjconv does not recognize periodic molecules	David van der Spoel	01/12/2018 11:05 AM	
2139	GROMACS	Feature	New	Normal	More precise/explicit documentation conventions		01/07/2018 11:54 PM	

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
2373	GROMACS	Bug	New	Low	gmx -nice can't work		01/04/2018 11:17 AM	
2362	TNG trajectory library	Bug	New	Normal	tng_*_of_particle_nr_get() functions return wrong result for structures with multiple molecule types		12/21/2017 11:51 AM	
1583	GROMACS	Bug	New	Normal	gmx msd with mol flag requires excessive memory		12/18/2017 03:34 PM	
2255	GROMACS	Bug	New	Normal	nstlist override stopped affecting the input parameter listing		12/17/2017 08:05 AM	
2252	GROMACS	Bug	New	Low	Memory allocation failures with large page sizes during PME tuning		12/14/2017 04:27 AM	
2039	GROMACS	Bug	New	Normal	mdrun -pinstride defaults are too confusing		12/13/2017 04:14 AM	
1811	GROMACS	Bug	New	Normal	Extrac build issues		12/13/2017 03:43 AM	
2217	GROMACS	Bug	New	Low	GPU emulation and separate PME ranks doesn't work properly		12/12/2017 11:50 AM	
2099	Support Platforms	Feature	New	High	sharing accounts/credentials		12/06/2017 08:11 PM	
2232	GROMACS	Bug	New	Normal	pdb2gmx can't form special bonds with terminal patched atoms		12/03/2017 01:35 PM	
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	
2254	GROMACS	Feature	New	Normal	GPU extensions for Google Tests		09/19/2017 05:01 PM	
2241	GROMACS	Bug	New	Low	refdata can segfault when reading		09/07/2017 11:57 AM	
2226	GROMACS	Feature	New	Normal	Harmonise commands for exit in make_ndx and distance		08/04/2017 12:24 PM	
2220	GROMACS	Feature	New	Normal	report relevant env var behaviour to console		07/31/2017 09:40 PM	
1836	Support Platforms	Bug	New	Normal	Support a way to retrigger part of matrix job		07/22/2017 12:30 AM	
2208	GROMACS	Bug	New	Normal	cuFFT linking		06/30/2017 01:58 PM	
2207	GROMACS	Feature	New	Normal	solvent excluded volume of large molecule with periodic boundary condition		06/16/2017 10:37 AM	
1948	GROMACS	Feature	New	Low	add warning when non-identical GPUs are used		06/12/2017 08:45 PM	
1309	Support Platforms	Task	New	Normal	Jenkins verification improvements		06/01/2017 02:34 PM	
2096	Support Platforms	Bug	New	Normal	Redmine internal error with special characters		05/31/2017 08:48 PM	
1854	GROMACS	Feature	New	Normal	Remove all cyclic dependencies		05/25/2017 08:34 AM	
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	
2158	GROMACS	Task	New	Normal	consider adding post-submit test that runs PME with 2xNN kernels		04/19/2017 08:04 PM	
2149	Support Platforms	Bug	New	Normal	gerrit server excessive CPU usage		04/05/2017 07:25 PM	
2020	GROMACS	Bug	New	Normal	Possible issue with md-vv integrator	Mark Abraham	03/11/2017 08:30 AM	

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
2133	GROMACS	Task	New	Low	gmx traj needs reform		03/07/2017 02:02 PM	
2118	GROMACS	Feature	New	Low	More verbose comments requested in header of gmx distance -oxyz		02/08/2017 05:46 AM	
2094	GROMACS	Bug	New	Normal	Solvation Consistency with MARTINI forcefield water across GROMACS versions with user-specified VDW size		01/20/2017 04:56 PM	
2101	GROMACS	Feature	New	Low	warninp could print the offending line, as well as its number		01/20/2017 03:06 PM	
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	
2090	GROMACS	Feature	New	Normal	redirecting stdout or stderr for testing	Mark Abraham	12/15/2016 03:15 AM	
2084	GROMACS	Task	New	Low	MPI and stderr/log output		11/28/2016 06:37 PM	
2080	GROMACS	Feature	New	Normal	add grompp warning for suitability for domain decomposition		11/23/2016 03:03 PM	
1829	GROMACS	Task	New	Normal	Future of thread level parallelism		11/18/2016 05:29 PM	
1026	GROMACS	Feature	New	Low	request for gen_vel to work with multiple temperature coupling groups at different temperatures		11/17/2016 04:39 PM	
2069	GROMACS	Task	New	Low	Simple thread-parallelism inside routines		11/09/2016 06:06 PM	
2060	GROMACS	Feature	New	Normal	Convert enum to enum class		10/17/2016 05:27 PM	
2056	GROMACS	Feature	New	Low	rename "gmx select"		10/03/2016 08:24 PM	
1105	Benchmark suite	Feature	New	Normal	produce a benchmark suite		09/13/2016 10:31 PM	
2048	GROMACS	Task	New	Normal	C++11: CUDA dependency on general headers		09/07/2016 10:30 PM	
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	
2015	GROMACS	Feature	New	Normal	Auto recovery from dd communication error		07/28/2016 03:17 PM	
2018	GROMACS	Feature	New	Normal	Pulling along a line between given points		07/27/2016 09:59 AM	
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	
948	GROMACS	Task	New	Normal	C++ thread synchronization primitives	Sander Pronk	07/11/2016 08:24 PM	
950	GROMACS	Feature	New	Normal	Path/directory/filename handling in Gromacs		07/11/2016 08:24 PM	
1017	GROMACS	Task	New	Normal	C++ Vector/Matrix classes		07/11/2016 08:23 PM	
1139	GROMACS	Feature	New	Normal	Adding the possibility to arbitrarily evaluate different components in the energy/force term when the energy/force is calculated		07/11/2016 08:19 PM	
1140	GROMACS	Task	New	Normal	Class design for passing options and data		07/11/2016 08:19 PM	
1303	GROMACS	Feature	New	Normal	Adding lambda dependent distance for pull code	Michael Shirts	07/11/2016 08:18 PM	
1498	GROMACS	Feature	New	Low	g_dipoles does not work properly with ionic systems	David van der Spoel	07/11/2016 08:11 PM	

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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	
1515	GROMACS	Task	New	Normal	improve g_bar output	Szilárd Páll	07/11/2016 08:10 PM	
1523	GROMACS	Task	New	Normal	add missing code-paths to CUDA emulation kernel		07/11/2016 08:09 PM	
1562	GROMACS	Feature	New	Normal	introducing a Monte Carlo framework (first application: MC barostat)	Michael Shirts	07/11/2016 08:08 PM	
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	
1658	GROMACS	Feature	New	Normal	Electrostatics treatment for multiple lambda sites	Berk Hess	07/11/2016 08:05 PM	
1849	GROMACS	Feature	New	Normal	expanded ensemble -- Adaptive Integration Method	Christopher Mirabzadeh	07/11/2016 08:01 PM	
1864	GROMACS	Feature	New	Normal	write tng files with energies	Magnus Lundborg	07/11/2016 08:00 PM	
1934	GROMACS	Bug	New	Normal	QMMM with ORCA: memory leaks, buffer overflows and much more		07/10/2016 09:26 AM	
2003	GROMACS	Task	New	Normal	reconsider various simd flags		07/07/2016 11:23 PM	
2001	GROMACS	Feature	New	Normal	add MPI info to the mdrun log header		07/06/2016 05:21 PM	
1855	GROMACS	Task	New	Normal	Convert preprocessor use so that symbols are always defined		06/28/2016 02:17 PM	
1667	GROMACS	Bug	New	Normal	gmx convert-tpr writes wrong number of mol in output tpr	David van der Spoel	06/27/2016 08:29 PM	
1670	GROMACS	Feature	New	Normal	create mdrun option checking mini-tool		06/23/2016 04:06 PM	
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	
1900	GROMACS	Feature	New	Normal	Implement some new errors in grompp		06/22/2016 05:20 PM	
1745	GROMACS	Task	New	Normal	Moving to C++11 after Gromacs-5.1		06/01/2016 03:01 PM	
1974	GROMACS	Feature	New	Normal	Report atom numbers and types in the error message about missed parameters		05/30/2016 09:24 AM	
1973	GROMACS	Task	New	Normal	OpenCL implementation wish list		05/27/2016 03:42 PM	
1568	GROMACS	Bug	New	Low	inconsistent/incorrect threading checks and reporting in mdrun		05/25/2016 02:01 AM	
1732	Support Platforms	Bug	New	Normal	review and extend jenkins tests setups, coverage		05/03/2016 05:30 AM	
1947	GROMACS	Task	New	Normal	Consider fixing corner case in TinyXML2	Mark Abraham	04/19/2016 01:40 AM	
1885	GROMACS	Feature	New	Normal	DPD Thermostat		01/26/2016 10:17 AM	
1867	GROMACS	Feature	New	Normal	make coupling implementations reversible		12/02/2015 07:43 AM	
1828	GROMACS	Task	New	Normal	Exception handling in mdrun		10/07/2015 11:36 AM	
1786	GROMACS	Task	New	Normal	Python style standards in developer docs	Peter Kasson	07/30/2015 05:45 PM	

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1770	GROMACS	Bug	New	Normal	segmentation fault with free energy changes and multiple GPU's		07/14/2015 03:24 AM	
1456	GROMACS	Task	New	Low	remove the use of nbat->alloc/free pointers	Szilárd Páll	06/20/2015 11:53 PM	
1246	GROMACS	Task	New	Normal	expanded ensemble .tpr cannot be rerun	Michael Shirts	06/19/2015 01:56 PM	
1635	GROMACS	Feature	New	Normal	Proper Unicode support		06/18/2015 08:34 PM	
1641	GROMACS	Feature	New	Normal	Add toolchain file for Cray systems		06/06/2015 11:24 PM	
1601	Support Platforms	Feature	New	Normal	use Git for Jenkins Config		05/24/2015 10:59 AM	
1688	GROMACS	Feature	New	Low	g_cluster "middle" is not exactly the same as the definition in the cited paper		04/01/2015 05:53 AM	
1490	GROMACS	Task	New	Normal	Usage of forward declarations vs typedef vs #include	Mark Abraham	01/21/2015 10:23 AM	
1655	GROMACS	Bug	New	Normal	g_membed and box type		12/09/2014 01:33 PM	
1634	GROMACS	Feature	New	Normal	Boxed Molecular Dynamics		11/04/2014 04:40 PM	
1602	GROMACS	Feature	New	Low	gmx order S per slice along all 3 axes		09/22/2014 07:25 AM	
1530	GROMACS	Task	New	Low	Offer binary downloads		06/29/2014 02:58 PM	
1508	Support Platforms	Task	New	Normal	Update master Jenkins build configurations		06/28/2014 03:59 AM	
1536	TNG trajectory library	Bug	New	Normal	TNG uses incorrect format for size_t on 32bit		06/28/2014 03:56 AM	
731	GROMACS	Feature	New	Normal	pdb2gmx should warn about missing residues when bonds are too long		06/22/2014 10:55 AM	
1102	GROMACS	Feature	New	Normal	Detect incompletely written itp files		06/19/2014 03:23 PM	
1106	Benchmark suite	Feature	New	Normal	publish benchmark numbers		06/19/2014 12:08 PM	
677	GROMACS	Task	New	Normal	Make sure manual uses consistent style throughout		06/19/2014 11:49 AM	
1190	GROMACS	Bug	New	Normal	Use of FORCE in setting cached variables	Mark Abraham	06/17/2014 06:09 AM	
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	
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	
1373	GROMACS	Task	New	Low	Add missing nbxn tests	Mark Abraham	06/09/2014 08:36 PM	
843	GROMACS	Feature	New	Low	g_helixorient could benefit from more documentation	Erik Lindahl	05/23/2014 02:02 PM	
1489	GROMACS	Feature	New	Normal	Don't solely rely on filename extension		04/30/2014 05:23 AM	
1214	GROMACS	Task	New	Normal	Keep track of important changes for Changelog	Mark Abraham	06/26/2013 11:24 AM	
1028	GROMACS	Feature	New	Normal	Tool to calculate fraction of native contacts during simulation		11/01/2012 10:27 PM	
987	Support Platforms	Feature	New	Normal	Feature wishlist should be moved to Redmine		08/03/2012 12:22 PM	
2107	GROMACS	Task	Accepted	High	Change to clang-format		08/02/2019 07:30 PM	
2702	GROMACS	Bug	Accepted	Normal	PME gather reduction race in OpenCL (and CUDA)		03/28/2019 03:14 PM	
1511	GROMACS	Feature	Accepted	Normal	add PDBx (ie mmcif) support		10/05/2018 07:14 PM	

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2448	GROMACS	Task	Accepted	Normal	should mdrun -multidir permit only one directory?		03/21/2018 12:10 PM	
2233	GROMACS	Bug	Accepted	Normal	replica exchange and -append bugged?		03/05/2018 01:38 PM	
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	
2194	GROMACS	Feature	Accepted	Low	xvg output requested as an output option in place of xpm files		05/31/2017 04:26 PM	
2166	GROMACS	Task	Accepted	Normal	gmx trjconv functionality should check for mismatch between the tpr and the trajectory		05/05/2017 04:32 PM	
1907	GROMACS	Task	Accepted	Low	keeping compile- and run-time CPU/arch detection consistent		08/01/2016 10:09 PM	
1056	GROMACS	Task	Accepted	Normal	status of fft5d_threads and fftw3_threads functionality	Mark Abraham	07/11/2016 08:21 PM	

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