

Issues

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
3202	GROMACS	Bug	New	Low	gmx solvate fails to overwrite topology file		11/13/2019 02:44 PM	
3201	GROMACS	Task	In Progress	Normal	Convert mdp parameters to key value tree		11/06/2019 06:06 PM	
3200	GROMACS	Bug	New	Normal	Segmentation Fault in gmx mdrun in gromacs 2020-beta1		11/13/2019 03:02 PM	2020-beta3
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	
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
3196	GROMACS	Bug	New	Normal	ExponentialMovingAverage.DeterminesCorrectlyIfIncreasing failing		11/01/2019 11:28 PM	
3195	GROMACS	Task	New	High	assess nightly master failures		11/01/2019 09:21 PM	2020-beta3
3194	GROMACS	Task	New	Normal	consider passing GPU dependency list to both dependency producers and consumers		11/01/2019 07:10 PM	
3188	GROMACS	Task	New	Normal	re-enable parallel spline calculation for #threads/atoms > 4		11/03/2019 09:18 PM	2020
3187	GROMACS	Task	New	Normal	Template updated PME kernels using threads per atom		10/30/2019 11:33 AM	
3186	GROMACS	Task	In Progress	Normal	Update Constant/Variable naming in the PME GPU kernels.		10/30/2019 11:23 AM	
3185	GROMACS	Task	New	Normal	Update PME CUDA kernels to allow a different number of threads per atom in the gather and spread kernels.		10/30/2019 11:18 AM	
3184	GROMACS	Bug	New	Normal	Cmdlineparser can't work with single-quoted atom names (typically used in DNA)		10/30/2019 08:49 AM	
3183	GROMACS	Task	Accepted	Normal	enable bonded interactions on GPU		10/31/2019 11:49 AM	2020-beta3
3182	GROMACS	Bug	New	Normal	pressure coupling buggy with GPU update		10/28/2019 11:34 PM	
3181	GROMACS	Task	New	Normal	consolidate task assignment and workload data initialization		10/28/2019 02:53 PM	
3177	GROMACS	Feature	New	Normal	Spack package management support		11/06/2019 06:37 PM	
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
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	
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
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

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3152	GROMACS	Feature	New	Low	Infrastructure and patterns for expressing public interfaces		10/17/2019 10:40 AM	2021-infrastructure-stable
3142	GROMACS	Feature	In Progress	High	centralize and clarify GPU force buffer clearing		11/01/2019 04:28 PM	2020-beta3
3138	GROMACS	Feature	New	Normal	Improve ensemble support in Context specification.		10/15/2019 03:56 PM	
3135	GROMACS	Feature	New	Normal	Make GPU traits into opaque types		10/14/2019 10:24 AM	
3132	GROMACS	Task	New	Normal	gmxapi testing support tools		10/31/2019 03:35 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	
3125	GROMACS	Bug	New	Normal	OpenCL on Volta and Turing broken		11/04/2019 11:37 AM	2020-beta3
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	
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
3119	GROMACS	Task	New	Normal	clang-tidy coverage of parallelization codepaths		10/04/2019 12:17 PM	2020
3115	GROMACS	Feature	New	Normal	Device stream manager		10/04/2019 09:00 AM	
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
3101	GROMACS	Bug	Blocked, need info	Normal	detect compilation failed		09/24/2019 05:26 PM	
3097	GROMACS	Bug	New	Normal	nbxnm grid issue with regressiontest complex/nbxnm_rzero with gpbufferops path		11/01/2019 03:22 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
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	
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	Feedback wanted	Normal	PME/PP GPU Comms unique pointer deletion causes seg fault when CUDA calls exist in destructor		11/01/2019 06:56 PM	
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	
3068	GROMACS	Bug	New	Normal	Misleading warning on rerun		08/26/2019 03:44 PM	

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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
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	
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	
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	
3037	GROMACS	Task	New	Normal	add missing cylcle counters related to buffer ops/reduction launches		09/24/2019 03:27 PM	2020
3033	GROMACS	Task	In Progress	Normal	Clean up and modernize googletest bundling and usage		08/24/2019 05:23 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	
3029	GROMACS	Feature	In Progress	High	GPU force buffer ops + reduction		11/01/2019 04:28 PM	2020-beta3
3028	GROMACS	Bug	Feedback wanted	Normal	install fail on Centos 6		07/15/2019 12:32 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	Resolved	Normal	modernized naming for new GPU developments		11/11/2019 01:03 PM	2020
3021	GROMACS	Feature	Feedback wanted	Normal	Completion of docs for GPU developments		11/01/2019 06:29 PM	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		11/01/2019 03:23 PM	2020-beta3
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 gmx_fatal		09/06/2019 02:34 PM	2021-infrastructure-stable
3014	GROMACS	Task	New	Normal	gmxapi example Python scripts		06/28/2019 11:07 AM	2020

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3013	GROMACS	Task	New	Normal	Extend logging levels in MDLogger		09/06/2019 02:34 PM	2021-infrastructure-stable
3010	GROMACS	Task	In Progress	Normal	upgrade OpenCL stack on bs-gpu01		10/29/2019 05:41 PM	2020-rc1
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 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	
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
2998	GROMACS	Task	In Progress	Normal	Update Python detection		10/29/2019 05:42 PM	2020-beta3
2997	GROMACS	Task	New	Normal	improve performance of alchemical free energy calculations		06/24/2019 03:07 PM	2020
2994	GROMACS	Feature	New	Normal	Data flow topology in gmxapi 2020		06/24/2019 01:53 PM	2020
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		11/01/2019 03:24 PM	2020-beta3
2988	GROMACS	Task	In Progress	Low	clean up and refactor code to modern standards		06/20/2019 02:14 PM	2020
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		11/08/2019 08:55 PM	2020
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		10/31/2019 03:35 PM	2020-beta3
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		11/01/2019 03:24 PM	2020-beta3
2957	GROMACS	Feature	New	Normal	add support for the Hygon Dhyana architecture		05/21/2019 01:00 PM	2020

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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	
2947	GROMACS	Task	Accepted	Normal	make an end to end test for membed		09/24/2019 03:22 PM	future
2937	TNG trajectory library	Bug	New	Normal	tng_num_frames_get reports incorrect num frames		04/29/2019 11:30 AM	
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
2935	Support Platforms	Bug	New	High	redmine issue updates about gerrit uploads stopped working		06/11/2019 01:42 PM	current
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	
2928	GROMACS	Feature	New	Normal	Add ability to use expression "count of ATOM_EXPR" in selection statements.		04/16/2019 04:52 PM	
2927	GROMACS	Bug	Feedback wanted	Low	CMake 3.14.1 fails to properly run gmxDetectCpu.make		11/12/2019 10:30 AM	2019.5
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	
2915	GROMACS	Feature	New	High	GPU direct communications		10/24/2019 10:59 AM	
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	
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	
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	
2896	GROMACS	Feature	In Progress	Normal	Python packaging		10/09/2019 04:08 PM	2020
2891	GROMACS	Feature	New	High	PME/PP GPU communications		11/01/2019 06:56 PM	
2890	GROMACS	Feature	New	High	GPU Halo Exchange		10/17/2019 02:00 PM	2020
2883	GROMACS	Bug	New	Normal	essentialdynamics fail with Intel MPI		03/08/2019 03:10 AM	
2873	GROMACS	Bug	New	Normal	Simple way to get last frame from trajectory		02/28/2019 11:14 PM	

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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	
2863	GROMACS	Task	New	Normal	improve PBC handling		03/11/2019 04:28 PM	
2862	GROMACS	Bug	In Progress	Normal	Division by zero in restrained dihedrals		04/01/2019 11:53 AM	2020
2860	GROMACS	Feature	New	Normal	Option for outputting min/max coordinates in gmx traj		02/08/2019 12:35 AM	
2859	GROMACS	Task	Fix uploaded	Normal	Change ArrayRef iterator type from pointer to std::iterator		02/08/2019 11:00 PM	
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	
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	
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	
2828	GROMACS	Bug	Feedback wanted	Normal	Installation issue on Power 9 system with SIMD support		01/18/2019 11:54 AM	
2817	GROMACS	Feature	In Progress	High	GPU X/F buffer ops		11/01/2019 04:28 PM	2020-beta3
2806	GROMACS	Feature	New	Normal	SIMD algorithms for ARM SVE // nobnonded cluster and others		12/12/2018 05:52 PM	2020
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	High	Improvement of PME gather and spread CUDA kernels		10/30/2019 01:29 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	
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
2763	GROMACS	Bug	New	Normal	GMXAPI layout / grouping in development docs "modules" page		12/14/2018 12:49 PM	future

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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	
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
2756	GROMACS	Task	In Progress	Normal	gmxapi integration testing		10/29/2019 05:38 PM	2020-beta3
2739	GROMACS	Feature	New	Normal	Parallel continuous tempering and enhanced sampling feature		11/13/2018 11:36 PM	
2728	GROMACS	Bug	New	Normal	Fix NB kernel picking		11/02/2018 03:51 PM	2020
2727	GROMACS	Task	In Progress	Low	Move non-analysis functions out of gmxana		01/20/2019 07:48 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
2713	GROMACS	Feature	New	Normal	Constant offset for external electric fields		10/28/2018 12:57 AM	
2710	GROMACS	Feature	New	Normal	Separate dvl 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	
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	
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	
2675	GROMACS	Task	In Progress	Normal	bonded CUDA offload task		10/29/2019 03:11 PM	2020
2674	GROMACS	Task	Accepted	Normal	Improve domain decomposition for bilayer systems		12/07/2018 04:03 PM	future
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	
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	
2643	GROMACS	Feature	New	Low	mdp options and/or docs for anisotropic aspects of implementations		09/12/2018 02:23 PM	

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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 versionc with cross-compilation enabled		12/03/2018 01:35 PM	future
2628	GROMACS	Bug	Fix uploaded	Normal	GMXRC removes trailing colon from existing MANPATH		08/28/2018 03:13 PM	
2624	GROMACS	Bug	New	Normal	GPU build system not robust enough		09/05/2018 02:00 AM	
2623	GROMACS	Task	Resolved	Normal	Allow extensible MDModules and forceProviders.		10/15/2018 03:44 PM	
2622	GROMACS	Feature	New	Low	Reduce severity of Berendsen warning		08/23/2018 11:16 PM	future
2620	GROMACS	Feature	In Progress	Normal	MD signaling API		03/02/2019 01:24 AM	
2616	GROMACS	Task	New	Normal	Model for MD state		09/14/2018 05:12 PM	
2615	GROMACS	Feature	Accepted	Normal	Switch to Python3		07/05/2019 02:57 PM	2020
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	
2602	GROMACS	Bug	New	Low	build information gets outdated if build tree is reused		08/13/2018 09:04 PM	
2600	GROMACS	Bug	New	High	coul-lambdas turns off all coulombic interactions in system instead of the molecule specified in the couple-moltype		08/07/2018 06:50 PM	
2598	GROMACS	Bug	New	Normal	Tools using read_next_x cannot read TNG files with sanitizers		10/15/2018 01:16 PM	future
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	
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	
2581	GROMACS	Feature	Accepted	Normal	User interface for hybrid Monte Carlo		10/15/2018 05:21 PM	2020
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	
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	
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	

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
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	
2555	GROMACS	Bug	New	Low	building GROMACS 2018.2		07/03/2018 11:41 PM	
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
2514	GROMACS	Task	New	Normal	PME OpenCL reductions with intrinsics		05/31/2018 12:27 AM	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	
2488	GROMACS	Task	New	Normal	use MPI non-blocking collectives to overlap pull comm		04/25/2018 04:19 PM	
2482	GROMACS	Bug	Feedback wanted	Normal	Atoms/molecules in freezegrps move and system crashes		05/18/2018 07:13 PM	
2481	GROMACS	Task	New	Low	Update gmx report-methods to write more method information		09/20/2018 07:43 AM	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	

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
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	
2448	GROMACS	Task	Accepted	Normal	should mdrun -multidir permit only one directory?		03/21/2018 12:10 PM	
2445	GROMACS	Task	New	Normal	Decide if/how to check for incompatible user input to mdrun for bonds and vsites		03/13/2018 02:02 PM	
2435	GROMACS	Task	New	Normal	identify and note about/tune task offload in GPU-bound runs		03/02/2018 04:08 PM	
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	
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
2422	GROMACS	Task	New	Normal	write C kernel for tables in Verlet scheme		02/26/2018 01:38 PM	
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
2393	GROMACS	Bug	New	Normal	incorrect error message with omitted command line flag before its argument		01/24/2018 11:24 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
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	
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
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	
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
2310	GROMACS	Feature	Accepted	Low	Let mdrun dump coordinates with non-finite energy		10/03/2018 09:47 PM	future

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
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	
2288	GROMACS	Feature	Accepted	Low	gmx msd doesn't optimally handle missing input trajectory frames		11/10/2017 11:03 AM	
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	
2240	GROMACS	Task	Accepted	Low	GPU emulation mode support for PME missing		09/16/2017 10:02 PM	
2239	GROMACS	Feature	New	Normal	split libgromacs into base and full		01/07/2019 01:47 AM	
2233	GROMACS	Bug	Accepted	Normal	replica exchange and -append bugged?		03/05/2018 01:38 PM	
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	
2226	GROMACS	Feature	New	Normal	Harmonise commands for exit in make_ndx and distance		08/04/2017 12:24 PM	
2221	GROMACS	Task	New	Normal	Avoid preprocessor for SIMD functions		02/21/2018 01:43 PM	
2220	GROMACS	Feature	New	Normal	report relevant env var behaviour to console		07/31/2017 09:40 PM	
2218	GROMACS	Feature	Feedback wanted	Normal	A tiny feature: damping for umbrella pull		08/16/2017 07:20 PM	
2217	GROMACS	Bug	New	Low	GPU emulation and separate PME ranks doesn't work properly		12/12/2017 11:50 AM	
2211	GROMACS	Bug	New	Low	gmx writes normal output to stderr		03/05/2018 02:00 PM	future
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	
2194	GROMACS	Feature	Accepted	Low	xvg output requested as an output option in place of xpm files		05/31/2017 04:26 PM	
2185	GROMACS	Task	New	Normal	add docs on MPI + CUDA w/wo MPS		05/24/2017 05:17 PM	
2182	GROMACS	Task	New	Low	de-duplicate code in densorder and hydorder		05/16/2017 11:29 AM	
2180	Support Platforms	Feature	Fix uploaded	Low	relog matrices would work better with a hint for execution		05/19/2017 01:02 AM	
2178	GROMACS	Task	New	Normal	Move checks for specific warnings to source repo		05/12/2017 03:57 PM	
2175	GROMACS	Task	New	Normal	improve clang static analyzer docs further		01/04/2018 04:13 PM	future
2169	GROMACS	Task	New	Normal	remove 'continuation' mdp option		10/12/2018 10:36 PM	2020
2168	GROMACS	Task	Feedback wanted	Normal	Design for multiple comparisons against same test reference data		05/08/2017 02:45 PM	future

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
2166	GROMACS	Task	Accepted	Normal	gmx trjconv functionality should check for mismatch between the tpr and the trajectory		05/05/2017 04:32 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	
2147	GROMACS	Bug	Feedback wanted	Normal	Parrinello-Rahman barostat not properly working		06/06/2017 07:53 AM	
2139	GROMACS	Feature	New	Normal	More precise/explicit documentation conventions		01/07/2018 11:54 PM	
2133	GROMACS	Task	New	Low	gmx traj needs reform		03/07/2017 02:02 PM	
2132	GROMACS	Feature	New	Normal	Intermediate code for xvg handling		03/08/2017 05:12 PM	future
2126	GROMACS	Feature	New	Normal	implement native CUDA support in CMake		10/29/2019 09:03 PM	
2118	GROMACS	Feature	New	Low	More verbose comments requested in header of gmx distance -oxyz		02/08/2017 05:46 AM	
2115	GROMACS	Task	New	Normal	trjconv does too many things, and combinations of them work poorly		10/02/2018 09:04 AM	
2113	GROMACS	Bug	New	Normal	Google tests and execution order		03/05/2018 02:05 PM	
2111	GROMACS	Feature	In Progress	Normal	Implement Gaussian screening of electrostatics		02/23/2019 12:33 PM	
2107	GROMACS	Task	Accepted	High	Change to clang-format		08/02/2019 07:30 PM	
2101	GROMACS	Feature	New	Low	warninp could print the offending line, as well as its number		01/20/2017 03:06 PM	
2099	Support Platforms	Feature	New	High	sharing accounts/credentials		12/06/2017 08:11 PM	
2097	GROMACS	Feature	New	Low	Move output of dhdl file entirely toedr, rather than having a separate text dhdl file		01/05/2017 05:21 PM	future
2096	Support Platforms	Bug	New	Normal	Redmine internal error with special characters		05/31/2017 08:48 PM	
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	
2092	GROMACS	Task	New	Normal	Tests running on GPU, and hardware assignment		12/19/2017 05:27 PM	future
2089	GROMACS	Task	New	Normal	Encourage code review		01/10/2017 12:03 AM	
2084	GROMACS	Task	New	Low	MPI and stderr/log output		11/28/2016 06:37 PM	
2080	GROMACS	Feature	New	Normal	add grompp warning for suitability for domain decomposition		11/23/2016 03:03 PM	
2069	GROMACS	Task	New	Low	Simple thread-parallelism inside routines		11/09/2016 06:06 PM	
2068	GROMACS	Feature	New	Normal	Access to low level classes		03/02/2019 01:37 AM	future
2065	GROMACS	Bug	New	Normal	thread-MPI internal errors		11/08/2018 03:43 PM	
2060	GROMACS	Feature	New	Normal	Convert enum to enum class		10/17/2016 05:27 PM	
2059	GROMACS	Task	In Progress	Normal	Separate different types of data in t_state		10/12/2018 10:36 PM	2020
2056	GROMACS	Feature	New	Low	rename "gmx select"		10/03/2016 08:24 PM	
2055	GROMACS	Task	New	Low	Wiki registration is broken		01/20/2017 11:31 AM	

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
2053	GROMACS	Task	New	Normal	refine notation in GPU code		09/04/2019 01:47 PM	2020
2048	GROMACS	Task	New	Normal	C++11: CUDA dependency on general headers		09/07/2016 10:30 PM	
2039	GROMACS	Bug	New	Normal	mdrun -pinstride defaults are too confusing		12/13/2017 04:14 AM	
2035	GROMACS	Task	New	Normal	A common trajectory analysis data exchange format		03/15/2017 05:46 PM	future
2018	GROMACS	Feature	New	Normal	Pulling along a line between given points		07/27/2016 09:59 AM	
2015	GROMACS	Feature	New	Normal	Auto recovery from dd communication error		07/28/2016 03:17 PM	
2010	GROMACS	Task	New	Normal	Use size_t instead of int for indexing		07/01/2018 07:57 AM	
2009	GROMACS	Task	New	Normal	improve command-line reporting of useful things		07/26/2016 12:54 PM	
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	
1994	GROMACS	Feature	New	Low	explore using JIT for CUDA		07/11/2016 10:20 PM	future
1985	GROMACS	Bug	Fix uploaded	Low	CUDA build system refactoring awaiting review		10/15/2018 05:21 PM	2020
1977	GROMACS	Bug	Feedback wanted	Low	warning: __WORDSIZE not defined		09/21/2018 06:19 PM	2020
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	
1972	GROMACS	Feature	New	Normal	external potential modules for refinement against experimental data		08/22/2018 05:03 PM	future
1971	GROMACS	Task	New	Normal	Removing buggy features vs. keeping workflows		01/19/2018 01:36 PM	future
1967	Support Platforms	Bug	Resolved	Normal	Documentation pages generated by Jenkins do not render properly		08/27/2016 02:04 AM	
1966	GROMACS	Feature	New	Low	Hydrogen mass repartiniog		05/25/2016 06:04 PM	future
1964	GROMACS	Feature	Accepted	Normal	"pull=no" should not produce warnings about "unknown" pull keywords		05/20/2016 02:37 PM	
1953	GROMACS	Feature	New	Low	use more regular polymorphism for GPU code		05/06/2016 10:06 PM	future
1948	GROMACS	Feature	New	Low	add warning when non-identical GPUs are used		06/12/2017 08:45 PM	
1936	GROMACS	Task	New	Normal	treat default-able mdp fields as strings		04/02/2016 10:32 PM	future
1934	GROMACS	Bug	New	Normal	QMMM with ORCA: memory leaks, buffer overflows and much more		07/10/2016 09:26 AM	
1925	GROMACS	Task	In Progress	Normal	remove concept of unilateral global communication		07/15/2019 06:42 PM	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	
1900	GROMACS	Feature	New	Normal	Implement some new errors in grompp		06/22/2016 05:20 PM	

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
1885	GROMACS	Feature	New	Normal	DPD Thermostat		01/26/2016 10:17 AM	
1879	GROMACS	Task	In Progress	Low	make the GROMACS OpenCL kernel work on Gallium		11/30/2018 05:46 PM	future
1876	GROMACS	Task	New	Normal	Reorganize vector input passed to core MD routines		06/01/2016 01:59 PM	future
1867	GROMACS	Feature	New	Normal	make coupling implementations reversible		12/02/2015 07:43 AM	
1862	GROMACS	Task	New	Normal	Fully replace t_topology by gmx_mtop_t		02/13/2019 04:53 PM	
1855	GROMACS	Task	New	Normal	Convert preprocessor use so that symbols are always defined		06/28/2016 02:17 PM	
1854	GROMACS	Feature	New	Normal	Remove all cyclic dependencies		05/25/2017 08:34 AM	
1852	GROMACS	Task	New	Normal	Remove group scheme		09/27/2019 03:13 PM	future
1842	GROMACS	Feature	New	Normal	Replace XML with JSON		01/18/2018 05:12 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
1836	Support Platforms	Bug	New	Normal	Support a way to retrigger part of matrix job		07/22/2017 12:30 AM	
1829	GROMACS	Task	New	Normal	Future of thread level parallelism		11/18/2016 05:29 PM	
1828	GROMACS	Task	New	Normal	Exception handling in mdrun		10/07/2015 11:36 AM	
1827	GROMACS	Bug	New	Low	cmake multi-configuration generator support partly broken		12/11/2017 05:20 PM	future
1826	GROMACS	Task	New	Normal	investigate non-optimal results with CPU-GPU balancing on AMD		09/16/2015 06:32 PM	
1815	Support Platforms	Task	In Progress	Normal	implement and execute plan for new releng machinery		10/15/2016 05:37 PM	
1811	GROMACS	Bug	New	Normal	Extrae build issues		12/13/2017 03:43 AM	
1785	GROMACS	Task	New	Low	no pV term written to energy file when pressure coupling is anisotropic		07/26/2015 01:47 PM	future
1770	GROMACS	Bug	New	Normal	segmentation fault with free energy changes and multiple GPU's		07/14/2015 03:24 AM	
1768	GROMACS	Task	New	Normal	decide future of command-line options vs env vars		11/03/2016 05:51 PM	future
1745	GROMACS	Task	New	Normal	Moving to C++11 after Gromacs-5.1		06/01/2016 03:01 PM	
1732	Support Platforms	Bug	New	Normal	review and extend jenkins tests setups, coverage		05/03/2016 05:30 AM	
1731	Support Platforms	Bug	In Progress	Normal	document jenkins configuration and set up means to track changes		05/31/2017 06:13 PM	
1730	GROMACS	Bug	New	Normal	gmx compare does not compare all fields of a .tpr		06/12/2015 09:33 PM	future
1729	GROMACS	Task	New	Normal	Resolve whether and how to resolve "state" variables stored in .tpr		05/13/2015 10:48 AM	future
1715	GROMACS	Feature	New	Low	improve cycle counting GPU sharing and multi-sim		08/03/2016 12:32 PM	future
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	
1670	GROMACS	Feature	New	Normal	create mdrun option checking mini-tool		06/23/2016 04:06 PM	
1665	GROMACS	Feature	New	Normal	improve free energy non-bonded kernel performance		08/26/2019 03:47 PM	future
1655	GROMACS	Bug	New	Normal	g_membed and box type		12/09/2014 01:33 PM	

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
1641	GROMACS	Feature	New	Normal	Add toolchain file for Cray systems		06/06/2015 11:24 PM	
1635	GROMACS	Feature	New	Normal	Proper Unicode support		06/18/2015 08:34 PM	
1634	GROMACS	Feature	New	Normal	Boxed Molecular Dynamics		11/04/2014 04:40 PM	
1627	GROMACS	Feature	In Progress	Normal	DPD integrator		07/11/2016 08:08 PM	
1625	GROMACS	Feature	New	Normal	Gromacs Python API		03/02/2019 01:44 AM	future
1602	GROMACS	Feature	New	Low	gmx order S per slice along all 3 axes		09/22/2014 07:25 AM	
1601	Support Platforms	Feature	New	Normal	use Git for Jenkins Config		05/24/2015 10:59 AM	
1587	GROMACS	Task	New	Normal	improve the configurability of regression tests		01/18/2019 06:17 AM	2020
1583	GROMACS	Bug	New	Normal	gmx msd with mol flag requires excessive memory		12/18/2017 03:34 PM	
1568	GROMACS	Bug	New	Low	inconsistent/incorrect threading checks and reporting in mdrun		05/25/2016 02:01 AM	
1551	Support Platforms	Bug	Feedback wanted	Normal	git index.lock issue		05/31/2017 05:37 PM	
1536	TNG trajectory library	Bug	New	Normal	TNG uses incorrect format for size_t on 32bit		06/28/2014 03:56 AM	
1530	GROMACS	Task	New	Low	Offer binary downloads		06/29/2014 02:58 PM	
1523	GROMACS	Task	New	Normal	add missing code-paths to CUDA emulation kernel		07/11/2016 08:09 PM	
1511	GROMACS	Feature	Accepted	Normal	add PDBx (ie mmcif) support		10/05/2018 07:14 PM	
1508	Support Platforms	Task	New	Normal	Update master Jenkins build configurations		06/28/2014 03:59 AM	
1489	GROMACS	Feature	New	Normal	Don't solely rely on filename extension		04/30/2014 05:23 AM	
1476	GROMACS	Bug	New	Low	Odd behavior with verlet-buffer-drift		05/25/2016 01:45 AM	future
1437	GROMACS	Feature	New	Normal	Online help formatting improvements		06/04/2015 09:20 PM	future
1328	GROMACS	Feature	Accepted	Normal	Names for selection positions		07/11/2016 08:15 PM	
1309	Support Platforms	Task	New	Normal	Jenkins verification improvements		06/01/2017 02:34 PM	
1221	GROMACS	Feature	Accepted	Normal	More generic position mapping for selections		06/10/2014 02:58 PM	future
1206	TNG trajectory library	Feature	New	Low	XTC Compression		10/25/2013 03:43 PM	version 2
1202	TNG trajectory library	Feature	New	Normal	Other hash types		06/25/2013 10:02 PM	version 2
1197	TNG trajectory library	Feature	New	Normal	Rework the molecule descriptions		03/18/2013 04:16 PM	version 2
1182	GROMACS	Feature	New	Normal	improve trajectory writing to support parallel I/O		05/13/2014 10:42 AM	future
1170	GROMACS	Task	New	Normal	mdlib reorganization		11/17/2016 03:47 PM	future
1165	GROMACS	Feature	Accepted	Low	Multi-SIMD binaries		01/23/2019 02:08 PM	2020
1140	GROMACS	Task	New	Normal	Class design for passing options and data		07/11/2016 08:19 PM	

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
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	
1120	GROMACS	Feature	New	Low	Make build work with multi-cogfiguration generators		06/03/2014 03:04 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	
1104	GROMACS	Feature	New	Low	Implement dihedral restraints		02/06/2013 07:04 PM	future
1102	GROMACS	Feature	New	Normal	Detect incompletely written itp files		06/19/2014 03:23 PM	
1083	GROMACS	Feature	In Progress	Normal	Improve collective error/warning/note handling in mdrun		07/11/2016 08:21 PM	
1028	GROMACS	Feature	New	Normal	Tool to calculate fraction of native contacts during simulation		11/01/2012 10:27 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	
1017	GROMACS	Task	New	Normal	C++ Vector/Matrix classes		07/11/2016 08:23 PM	
988	GROMACS	Task	New	Normal	Definition of "public API"		08/28/2019 02:50 PM	future
987	Support Platforms	Feature	New	Normal	Feature wishlist should be moved to Redmine		08/03/2012 12:22 PM	
986	GROMACS	Task	New	Normal	Handling C++ out-of-memory errors		12/24/2014 08:42 PM	future
951	GROMACS	Feature	New	Normal	Multiple versions of Gromacs (e.g., single and double) in the same library/binary		01/07/2019 02:10 AM	future
950	GROMACS	Feature	New	Normal	Path/directory/filename handling in Gromacs		07/11/2016 08:24 PM	
921	GROMACS	Feature	Blocked, need info	Normal	Default index groups and selections		07/11/2016 08:27 PM	
909	GROMACS	Task	New	Normal	Reimplement displacement calculation module		07/14/2014 11:30 AM	future
907	GROMACS	Feature	Accepted	Normal	Add tests for verifying installed headers		03/11/2014 09:15 PM	future
895	GROMACS	Feature	In Progress	Normal	g_rmsf previous frame as reference		04/29/2013 07:39 PM	future
838	GROMACS	Task	New	Normal	Improve generic error reporting routines		07/11/2016 08:29 PM	
837	Support Platforms	Task	Resolved	Low	Consider subproject organization of the Gromacs project		07/14/2014 12:07 PM	
742	GROMACS	Feature	New	Normal	Enhancing the performance of the free energy code		08/26/2019 04:55 PM	future
731	GROMACS	Feature	New	Normal	pdb2gmx should warn about missing residues when bonds are too long		06/22/2014 10:55 AM	
720	GROMACS	Feature	Accepted	Low	permit pdb2gmx to choose a kind of HIS based on proton position		11/17/2016 03:51 PM	future
701	GROMACS	Task	New	Normal	Add symbol visibility macros		03/02/2019 01:46 AM	future
687	Support Platforms	Feature	New	Normal	Add content on the front page		09/02/2019 01:08 PM	
677	GROMACS	Task	New	Normal	Make sure manual uses consistent style throughout		06/19/2014 11:49 AM	
665	GROMACS	Task	New	Normal	Port existing trajectory analysis tools to use the new framework		07/14/2014 11:29 AM	future
652	GROMACS	Task	Blocked, need info	Normal	Change selection method implementation to use C++		04/23/2017 08:05 PM	future

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
3164	GROMACS	Bug	New	High	mdrun-mpi-test with separate PME ranks and PP-PME CPU comm crashes	Alan Gray	11/13/2019 08:23 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
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
3158	GROMACS	Task	In Progress	Normal	use MPI_Isend() in sendFTToPpCudaDirect and receiveCoordinatesFromPpCudaDirect	Alan Gray	11/07/2019 05:26 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
3106	GROMACS	Task	New	Normal	Implement multiple pulses with GPU communication	Alan Gray	11/01/2019 11:05 AM	future
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
2537	GROMACS	Task	New	Normal	Simplify PME solve reduction	Aleksei lupinov	10/30/2018 12:08 PM	2020
2516	GROMACS	Task	New	Low	Support PME OpenCL execution width < 16	Aleksei lupinov	06/05/2019 05:32 PM	
2453	GROMACS	Task	Resolved	High	PME OpenCL porting effort	Aleksei lupinov	06/05/2019 05:32 PM	2020
2054	GROMACS	Feature	Accepted	High	PME on GPU	Aleksei lupinov	10/03/2019 09:41 PM	2020
438	GROMACS	Feature	In Progress	Low	New tool: g_correl	Alexey Shvetsov	06/20/2014 10:38 AM	future
3180	GROMACS	Task	New	Normal	Remove extra D2H and H2D copies of coordinates when the COM motion is compensated.	Artem Zhmurov	10/27/2019 10:48 AM	
3163	GROMACS	Bug	New	High	gpuupdate / task assignment stabilization	Artem Zhmurov	10/31/2019 03:35 PM	2020-beta3
3155	GROMACS	Task	Accepted	Normal	Unify DD and CPU-GPU gather & scatter	Artem Zhmurov	10/17/2019 03:50 PM	2021-infrastructure-stable
3114	GROMACS	Task	New	Low	Possible improvements to update-constraints	Artem Zhmurov	10/07/2019 11:38 AM	
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
2864	GROMACS	Task	New	Normal	Building incompatibilities	Benson Muite	02/19/2019 02:00 PM	

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
2755	GROMACS	Feature	New	Low	md5 sums and sha256, sha512 hashes	Benson Muite	02/19/2019 11:00 PM	
2596	GROMACS	Feature	New	Normal	Constant potential method	Benson Muite	05/10/2019 09:54 AM	
3173	GROMACS	Bug	Resolved	Normal	Illegal memory access in free-energy calculations	Berk Hess	10/23/2019 01:30 PM	2019.5
2979	GROMACS	Task	Accepted	Normal	Reconsider default 1 OpenMP thread per thread-MPI rank	Berk Hess	11/01/2019 03:24 PM	2020-rc1
2908	GROMACS	Task	New	Normal	Renaming things in nbxnm	Berk Hess	03/28/2019 10:10 AM	
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 nbxnm a module	Berk Hess	01/03/2019 03:07 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
2553	GROMACS	Bug	Accepted	Normal	Incorrect COM velocity correction with frozen atoms	Berk Hess	12/03/2018 01:15 PM	2020
2452	GROMACS	Task	In Progress	Normal	Reduce data dependencies in mdrun algorithms	Berk Hess	03/14/2018 08:47 PM	
2391	GROMACS	Task	Accepted	Normal	re-enable TPI test	Berk Hess	01/09/2019 05:17 PM	2020
2238	GROMACS	Task	In Progress	Normal	GPU emulation mode support for rolling pruning missing	Berk Hess	12/21/2017 03:21 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
2071	GROMACS	Task	In Progress	High	Low accuracy default settings yield incorrect liquid densities	Berk Hess	01/05/2018 03:32 PM	

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