

Issues

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
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	
3206	GROMACS	Bug	New	Normal	2 not-critical bugs in analyse tool		11/15/2019 03:53 PM	2019.5
3205	GROMACS	Task	New	High	address Debian experimental issues		11/18/2019 11:17 AM	2020-beta3
3204	GROMACS	Bug	In Progress	Normal	intermolecular interactions on OpenMPI multiple threads (gromacs 2019.4)	Berk Hess	11/17/2019 03:56 PM	2019.5
3203	GROMACS	Bug	Fix uploaded	Normal	Segmentation fault using gmx solvent	Paul Bauer	11/16/2019 06:27 PM	2019.5
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	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
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	
3193	GROMACS	Bug	New	Normal	Unused parameter warnings in pme code	Paul Bauer	11/01/2019 09:40 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
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	
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	
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	
3179	GROMACS	Feature	New	Normal	Clarify access to parallel data outputs	Eric Irrgang	10/26/2019 12:23 PM	

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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
3177	GROMACS	Feature	New	Normal	Spack package management support		11/06/2019 06:37 PM	
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
3174	GROMACS	Task	Feedback wanted	Low	Proposed gmxapi syntax update: "input" and "output" key word arguments -> "inputs" and "outputs"	Eric Irrgang	10/23/2019 06:34 PM	
3173	GROMACS	Bug	Resolved	Normal	Illegal memory access in free-energy calculations	Berk Hess	10/23/2019 01:30 PM	2019.5
3172	GROMACS	Feature	New	Normal	QM/MM Interface with CP2K	Dmitry Morozov	10/22/2019 12:35 PM	future
3171	GROMACS	Task	New	Normal	schedule CPU H2D force contribution in separate stream		10/22/2019 12:19 AM	2020
3170	GROMACS	Task	New	Low	investigate GPU f buffer ops use cases		10/22/2019 12:14 AM	2020
3168	GROMACS	Feature	New	Normal	GPU update release notes		11/14/2019 06:03 PM	2020-rc1
3167	GROMACS	Task	New	Normal	GPU update path user documentation		10/21/2019 04:09 PM	2020-beta3
3166	GROMACS	Bug	New	Normal	Compilation failing on Ubuntu 19.04 with Cuda 10.1		10/19/2019 09:13 PM	
3165	GROMACS	Bug	New	Normal	task assignment silent abort		10/18/2019 07:46 PM	
3164	GROMACS	Bug	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
3163	GROMACS	Bug	New	High	gpuupdate / task assignment stabilization	Artem Zhmurov	11/14/2019 06:01 PM	2020-beta3
3162	GROMACS	Feature	New	Normal	Add virtual site support to GPU version of update-constraints.		10/21/2019 03:59 PM	
3161	GROMACS	Bug	New	Normal	mdrun-test hangs with -ntmpi2		10/17/2019 05:34 PM	2020
3160	GROMACS	Feature	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
3155	GROMACS	Task	Accepted	Normal	Unify DD and CPU-GPU gather & scatter	Artem Zhmurov	10/17/2019 03:50 PM	2021-infrastructure-stable
3154	GROMACS	Task	New	Low	Update use of Python subprocess for >=3.5		10/17/2019 01:46 PM	
3153	GROMACS	Task	New	Low	Let CMake process module directories earlier to support more modern CMake idioms.		10/17/2019 10:40 AM	2021-infrastructure-stable
3152	GROMACS	Feature	New	Low	Infrastructure and patterns for expressing public interfaces		10/17/2019 10:40 AM	2021-infrastructure-stable
3150	GROMACS	Bug	New	Normal	gmxapi data type annotations are confusing and inadequate	Eric Irrgang	10/22/2019 03:08 PM	2021-infrastructure-stable
3149	GROMACS	Feature	New	Normal	Python user interface for obtaining simulation artifacts as files.	Eric Irrgang	10/15/2019 06:21 PM	

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3148	GROMACS	Feature	New	Normal	Roadmap for gmxapi filesystem interactions.	Eric Irgang	10/15/2019 06:23 PM	2021-infrastructure-stable
3147	GROMACS	Feature	New	Normal	gmxapi workflow checkpointing	Eric Irgang	10/15/2019 06:18 PM	2021-infrastructure-stable
3143	GROMACS	Task	New	Normal	move the non-force accumulation/accounting tasks out of the GPU wait functions	Szilárd Páll	10/14/2019 05:14 PM	2020
3142	GROMACS	Feature	In Progress	High	centralize and clarify GPU force buffer clearing		11/01/2019 04:28 PM	2020-beta3
3141	GROMACS	Bug	New	Normal	gmxapi File placeholders missing from beta release	Eric Irgang	10/15/2019 03:57 PM	2020
3140	GROMACS	Feature	New	Normal	Allow explicit input definition for gmxapi.operation function wrapper	Eric Irgang	10/15/2019 03:56 PM	2020
3139	GROMACS	Task	New	Normal	gmxapi Futures should be subscribable	Eric Irgang	10/15/2019 03:56 PM	
3138	GROMACS	Feature	New	Normal	Improve ensemble support in Context specification.		10/15/2019 03:56 PM	
3136	GROMACS	Bug	New	Normal	gmxapi.operation data flow topology unclear or incomplete	Eric Irgang	10/22/2019 03:09 PM	2020-beta3
3135	GROMACS	Feature	New	Normal	Make GPU traits ino opaque types		10/14/2019 10:24 AM	
3134	GROMACS	Feature	Feedback wanted	Normal	gmxapi Python exception names may need improvement	Eric Irgang	10/13/2019 01:50 PM	
3133	GROMACS	Task	New	Normal	Cookiecutter for sample_restraint	Eric Irgang	10/13/2019 01:07 PM	2020
3132	GROMACS	Task	New	Normal	gmxapi testing support tools		10/31/2019 03:35 PM	
3131	GROMACS	Task	New	Normal	support ccache with clang-tidy	Mark Abraham	10/29/2019 05:41 PM	2020-rc1
3130	GROMACS	Task	New	Normal	Interim handling of gmxapi data references.	Eric Irgang	10/22/2019 03:09 PM	2020-beta3
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 borken		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 parallelizaton codepaths		10/04/2019 12:17 PM	2020
3117	GROMACS	Feature	New	Normal	Coulomb FEP PME on GPU	Magnus Lundborg	10/04/2019 09:16 AM	future
3116	GROMACS	Bug	New	Normal	regressiontests/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	
3114	GROMACS	Task	New	Low	Possible improvements to update-constraints	Artem Zhmurov	11/14/2019 06:06 PM	
3113	GROMACS	Bug	New	Low	Use of read_tps_conf is depecrated	Paul Bauer	10/01/2019 11:36 AM	2021-infrastructure-stable
3106	GROMACS	Task	New	Normal	Implement multiple pulses with GPU communication	Alan Gray	11/01/2019 11:05 AM	future

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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	nbnxm grid issue with regressiontest complex/nbnxn_rzero with gpubufferops path		11/01/2019 03:22 PM	2020-beta3
3096	GROMACS	Task	New	Normal	Multiple time-stepping: correct coupling algorithms, virial calculation and energy output	Christian Blau	09/18/2019 02:18 PM	2021-infrastructure-stable
3093	GROMACS	Task	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	
3076	GROMACS	Task	New	Normal	Selectively activate MdModules during simulation instead of instantiating all of them	Christian Blau	09/05/2019 11:36 AM	2021-infrastructure-stable
3075	GROMACS	Bug	New	Normal	Frozen atoms are moving		09/04/2019 08:00 PM	
3073	GROMACS	Bug	New	Normal	Total potential energy goes crazy, but I don't know why this happens.		09/04/2019 07:25 PM	
3072	GROMACS	Task	New	Normal	Use gmx::index for indexing instead of int	Christian Blau	09/03/2019 04:23 PM	2021-infrastructure-stable
3071	GROMACS	Bug	Accepted	Normal	complex.nbnxn-ljpme-LB-geometric failing with OpenCL timing debug mode assertions	Szilárd Páll	09/02/2019 10:19 PM	2020
3069	GROMACS	Feature	New	Low	Iterator over span and indices into this span (zip-style iterator)	Christian Blau	08/29/2019 11:11 AM	future
3068	GROMACS	Bug	New	Normal	Misleading warning on rerun		08/26/2019 03:44 PM	
3066	GROMACS	Bug	New	Normal	Gauss transform and density fit classes should operate on real values instead of float	Christian Blau	08/26/2019 11:53 AM	
3064	GROMACS	Task	New	Normal	add test for perturbed bonded forces		08/22/2019 06:34 PM	2020
3062	GROMACS	Task	New	Normal	add twin cut-off mdrun test		08/19/2019 06:21 PM	2020
3058	GROMACS	Bug	Feedback wanted	Normal	Error when using a large PME grid on a GPU		09/04/2019 07:26 PM	
3057	GROMACS	Task	New	Normal	re-enable fusion on Power8/9	Szilárd Páll	08/12/2019 11:41 AM	2020
3055	GROMACS	Bug	Feedback wanted	Normal	Error in gmx xpm2ps		08/22/2019 03:27 PM	

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3054	GROMACS	Bug	New	Normal	Missing dihedral define		08/02/2019 05:47 PM	
3052	GROMACS	Feature	New	Normal	GPU virial reduction/calculation		08/01/2019 05:26 PM	
3050	GROMACS	Bug	New	Low	Fix tests on Solaris	Vedran Miletic	07/29/2019 12:38 PM	2020
3049	GROMACS	Bug	New	Low	gmx nmeig should plot a real infrared spectrum	David van der Spoel	09/24/2019 03:25 PM	future
3048	GROMACS	Bug	New	Normal	Dihedral parameters for N-terminal in gromos53a6 force field in the aminoacids.n.tdb file with different values in versions 4.6.7 and gromacs 2019/2016/5.1.5		07/29/2019 10:41 AM	
3047	GROMACS	Task	New	Normal	Set required versions for GROMACS 2021		08/24/2019 05:25 PM	2021-infrastructure-stable
3045	GROMACS	Feature	New	Low	Option to remove v-sites in trjconv?		07/19/2019 04:42 PM	
3042	GROMACS	Bug	New	Normal	core dump error in grompp command		10/09/2019 07:30 PM	
3041	GROMACS	Task	New	Normal	Remove workaround for gcc bug 58265		07/23/2019 12:27 PM	
3040	GROMACS	Task	New	Normal	Refactor Restraint module		07/18/2019 03:59 PM	
3038	GROMACS	Feature	New	Normal	Improvements to MD plugin development environment	Eric Irrgang	07/17/2019 02:15 PM	2020
3037	GROMACS	Task	New	Normal	add missing cylcle counters related to buffer ops/reduction launches		09/24/2019 03:27 PM	2020
3035	GROMACS	Task	New	Normal	Provide central logger in wrapper binary	Paul Bauer	09/06/2019 02:34 PM	2021-infrastructure-stable
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	
3027	GROMACS	Task	In Progress	Normal	Move sample_restraint development from GitHub to Gerrit	Eric Irrgang	11/01/2019 03:23 PM	2020-beta3
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
3013	GROMACS	Task	New	Normal	Extend logging levels in MDLogger		09/06/2019 02:34 PM	2021-infrastructure-stable

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3010	GROMACS	Task	In Progress	Normal	upgrade OpenGL 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
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
2993	GROMACS	Feature	New	Normal	Scalar and structured type expression and definitions for API	Eric Irrgang	10/17/2019 09:55 AM	
2992	GROMACS	Task	New	Normal	Split hw_opt in const user options and dynamic settings		09/24/2019 03:23 PM	2020
2990	GROMACS	Bug	New	Normal	ARM neon SIMD4 error		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
2984	GROMACS	Feature	New	Normal	More Extensive Selections Examples	Dallas Warren	06/18/2019 11:50 PM	
2983	GROMACS	Task	New	Normal	better suited data-types for bonded GPU kernels		07/11/2019 04:32 PM	
2981	GROMACS	Bug	New	Normal	segfault in opencl build		06/18/2019 03:30 AM	
2980	GROMACS	Bug	New	Normal	taskassignment fails with unit tests when GPUs and custom number of ranks is used		06/17/2019 05:28 PM	
2979	GROMACS	Task	Accepted	Normal	Reconsider default 1 OpenMP thread per thread-MPI rank	Berk Hess	11/01/2019 03:24 PM	2020-rc1
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

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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
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
2945	GROMACS	Task	New	Normal	Give MdModules access to simulation resources (e.g. atom selection manager or communication infrastructure)	Christian Blau	05/19/2019 01:26 PM	2020
2944	GROMACS	Feature	New	Normal	Roadmap for thermostats / barostats in new propagation/integration scheme	Michael Shirts	05/08/2019 05:50 PM	2020
2943	GROMACS	Task	New	Normal	Rename Integrator	Pascal Merz	05/23/2019 08:04 PM	2020
2936	GROMACS	Task	New	Normal	introduce check that CPU-GPU transfers are made between arrays of compatible types		05/13/2019 09:23 AM	2020
2934	GROMACS	Feature	New	Normal	GPU X Buffer ops		09/24/2019 06:07 PM	2020
2933	GROMACS	Task	New	Normal	Convert walls to a ForceProvider		04/25/2019 02:43 PM	
2931	GROMACS	Feature	New	Normal	Tables in Verlet kernels		04/29/2019 12:01 PM	
2930	GROMACS	Feature	New	Normal	Limited range for reference group detection in cylinder pulling		04/26/2019 05:17 PM	
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
2925	GROMACS	Bug	New	Normal	BasicVector addition operator yields unexpected result when adding scalar	Christian Blau	04/20/2019 05:39 PM	2020
2924	GROMACS	Bug	New	Normal	Failing version check when reading new tpr file with older gromacs version		04/12/2019 10:52 AM	
2919	GROMACS	Task	New	Normal	C++ style guidelines for namespace use		04/15/2019 01:21 PM	
2916	GROMACS	Task	New	Normal	Decide future of symtab	Paul Bauer	09/06/2019 02:35 PM	2021-infrastructure-stable
2915	GROMACS	Feature	New	High	GPU direct communications		10/24/2019 10:59 AM	
2912	GROMACS	Task	Resolved	Normal	C++ extension module for Python bindings	Eric Irrgang	07/05/2019 09:00 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	
2908	GROMACS	Task	New	Normal	Renaming things in nbnxm	Berk Hess	03/28/2019 10:10 AM	

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2907	GROMACS	Bug	New	Normal	Gromacs autocompletion appears to be broken with ZSH		07/16/2019 04:46 AM	
2905	GROMACS	Task	New	Normal	Add a Jenkins configuration with std library assert		08/24/2019 05:22 PM	
2902	GROMACS	Bug	New	Normal	2019.1 equilibration issue? (Intel 2018u3)		04/30/2019 08:17 AM	
2901	GROMACS	Feature	New	Normal	Declare external Resources in mdp / tpr files.	Christian Blau	03/27/2019 04:27 PM	2020
2898	GROMACS	Task	New	Low	Naming common variables		03/26/2019 11:46 PM	
2897	GROMACS	Bug	New	Normal	rotation/flex2 can still fail on cpu-only run on OpenCL build		04/04/2019 06:24 PM	
2896	GROMACS	Feature	In Progress	Normal	Python packaging		10/09/2019 04:08 PM	2020
2895	GROMACS	Task	Resolved	Normal	gmxapi Output proxy establishes execution dependency.	Eric Irrgang	03/29/2019 05:18 PM	2020
2894	GROMACS	Task	Resolved	Normal	Wrap importable Python code.	Eric Irrgang	05/09/2019 11:30 AM	2020
2893	GROMACS	Task	Resolved	Normal	Integrate gmxapi Python package	Eric Irrgang	10/23/2019 09:16 AM	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
2889	GROMACS	Task	New	Normal	update grompp warnings for brevity, usefulness and actionability	Mark Abraham	03/11/2019 02:15 PM	2020
2888	GROMACS	Feature	New	High	CUDA Update and Constraints module	Artem Zhmurov	10/21/2019 03:59 PM	2020
2887	GROMACS	Feature	New	Normal	CUDA version of Leap Frog algorithm	Artem Zhmurov	10/02/2019 12:00 PM	2020
2886	GROMACS	Feature	New	Normal	CUDA version of SETTLE	Artem Zhmurov	10/02/2019 12:02 PM	2020
2885	GROMACS	Feature	New	Normal	CUDA version of LINCS	Artem Zhmurov	03/12/2019 01:33 PM	2020
2883	GROMACS	Bug	New	Normal	essentialdynamics fail with Intel MPI		03/08/2019 03:10 AM	
2882	GROMACS	Task	New	Normal	evaluate different storage layouts for GPU coordinates/changes/forces	Szilárd Páll	03/07/2019 06:21 PM	
2877	GROMACS	Task	New	Normal	use gmx::Options more	Mark Abraham	04/02/2019 06:14 PM	2020
2876	GROMACS	Bug	New	Normal	2019.1 make check fails on AVX and AVX2 (Intel 2018u3)	Erik Lindahl	03/08/2019 10:32 AM	
2875	GROMACS	Task	Accepted	Normal	SIMD version of the free-energy kernel	Berk Hess	08/26/2019 03:47 PM	2020
2874	GROMACS	Task	New	Normal	Refactor Gromacs (cluster) neighborlist into separate module	Erik Lindahl	02/28/2019 11:36 AM	
2873	GROMACS	Bug	New	Normal	Simple way to get last frame from trajectory		02/28/2019 11:14 PM	
2872	GROMACS	Bug	New	Normal	gmx solvate and genion topology update		02/27/2019 10:18 AM	
2870	GROMACS	Bug	New	Normal	GPU detection error message missing from the output		03/05/2019 03:55 PM	
2869	GROMACS	Bug	New	Normal	GPU detection error only issued as a note to the log		03/05/2019 04:09 PM	
2866	GROMACS	Feature	New	Normal	Alternative non-bonded potentials	David van der Spoel	03/05/2019 03:50 PM	future

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
2864	GROMACS	Task	New	Normal	Building incompatibilities	Benson Muite	02/19/2019 02:00 PM	
2863	GROMACS	Task	New	Normal	improve PBC handling		03/11/2019 04:28 PM	
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	
2854	GROMACS	Bug	New	Normal	OnlineHelpUnitTests segfaults on s390x with gcc-9.0.1	Paul Bauer	02/04/2019 11:17 AM	
2853	GROMACS	Bug	New	Normal	EwaldUnitTests segfault on armv7hl with gcc-9.0.1	Paul Bauer	02/04/2019 05:34 PM	
2852	GROMACS	Bug	New	Low	the in-tree regressiontest download can get out of sync with code		01/30/2019 03:58 PM	
2850	GROMACS	Task	In Progress	Normal	assess Raptor Talos for testing	Szilárd Páll	02/12/2019 01:14 PM	
2848	GROMACS	Bug	New	Normal	gmx make_ndx ignores last residue in case only CA's are present in GRO file		01/30/2019 06:16 AM	
2846	GROMACS	Feature	New	Low	Set rpath in FindLibStdCpp.cmake		02/02/2019 08:09 AM	
2840	GROMACS	Feature	New	Normal	Test that functionality does not compile that is not supposed to.		01/25/2019 02:35 PM	future
2839	GROMACS	Task	New	Normal	make module and file naming consistent		04/09/2019 04:27 PM	2020
2835	GROMACS	Task	New	Normal	Matrix class constraint to upper or lower triangle		02/07/2019 02:44 PM	
2834	GROMACS	Task	New	Normal	C++ matrix classes	Christian Blau	01/23/2019 12:19 PM	2020
2833	GROMACS	Task	New	Normal	Update topology datastructures	Paul Bauer	04/02/2019 12:39 PM	2020
2832	GROMACS	Bug	New	Low	PaddedVector move operations broken	Mark Abraham	02/12/2019 03:22 PM	2020
2828	GROMACS	Bug	Feedback wanted	Normal	Installation issue on Power 9 system with SIMD support		01/18/2019 11:54 AM	
2822	GROMACS	Task	Accepted	Normal	Make nbxn a module	Berk Hess	01/03/2019 03:07 PM	2020
2818	GROMACS	Task	In Progress	Normal	bonded GPU kernel fusion	Magnus Lundborg	07/03/2019 09:01 PM	
2817	GROMACS	Feature	In Progress	High	GPU X/F buffer ops		11/01/2019 04:28 PM	2020-beta3
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
2806	GROMACS	Feature	New	Normal	SIMD algorithms for ARM SVE // nobonded cluster and others		12/12/2018 05:52 PM	2020
2798	GROMACS	Bug	New	Normal	Default mpi rank number fails when there are 16 cores and 3 gpus	Berk Hess	12/11/2018 10:11 PM	2020
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	

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
2791	GROMACS	Feature	In Progress	Normal	Implement a module for lambda-dynamics simulations (lambda_site module)	Thomas Ullmann	03/01/2019 01:36 AM	future
2788	GROMACS	Bug	New	Normal	PME will not run on AMD GPU with NVidia GPU present		01/03/2019 02:24 PM	
2787	GROMACS	Task	New	Normal	allow passing flags to allocateDeviceBuffer		12/03/2018 01:54 PM	
2785	GROMACS	Bug	New	Normal	Inconsistent and erroneous behaviour of trjconv when writing a partial TNG		11/30/2018 02:36 PM	
2774	GROMACS	Feature	New	Normal	Refactor shell code into its own integrator	David van der Spoel	03/29/2019 05:20 PM	2020
2773	GROMACS	Task	New	Normal	improve GPU error handling and make such handling uniform across modules		11/21/2018 10:28 AM	2020
2771	GROMACS	Task	New	Normal	Size independent Hessian for normal mode analysis		12/08/2018 08:06 PM	2020
2770	GROMACS	Task	New	Normal	change branch maintenance policy		11/29/2018 02:51 PM	2020
2767	GROMACS	Bug	New	Normal	grompp warns about md + FEP even for fully coupled states		11/19/2018 11:41 AM	2020
2766	GROMACS	Task	In Progress	Normal	Improve hardware option selection	Kevin Boyd	12/20/2018 06:40 PM	2020
2764	GROMACS	Task	New	Normal	gmxapi version updates for post release-2019	Eric Irrgang	11/21/2018 12:53 PM	
2763	GROMACS	Bug	New	Normal	GMXAPI layout / grouping in development docs "modules" page		12/14/2018 12:49 PM	future
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
2755	GROMACS	Feature	New	Low	md5 sums and sha256, sha512 hashes	Benson Muite	02/19/2019 11:00 PM	
2754	GROMACS	Bug	New	Normal	Simulated Tempering seems to be broken	Michael Shirts	02/05/2019 03:58 PM	
2740	GROMACS	Bug	New	Normal	mdrun reports incorrect error with -bonded gpu without gpu	Mark Abraham	11/07/2018 01:59 PM	
2739	GROMACS	Feature	New	Normal	Parallel continuous tempering and enhanced sampling feature		11/13/2018 11:36 PM	
2737	GROMACS	Bug	Accepted	Low	AMD OpenCL fails release build in complex tests	Szilárd Páll	11/01/2019 03:25 PM	2020-beta3
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
2734	GROMACS	Bug	In Progress	Normal	regressiontests/kernel core dumps on ppc64le	Paul Bauer	06/15/2019 04:12 PM	future
2733	GROMACS	Bug	Blocked, need info	Normal	MdrunUtilityMpiUnitTests timeout on i686 and armv7hl with OpenMPI 2.1.5	Paul Bauer	11/08/2018 04:27 PM	
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
2727	GROMACS	Task	In Progress	Low	Move non-analysis functions out of gmxana		01/20/2019 07:48 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

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
2722	GROMACS	Bug	New	Normal	gmxapi may over-manage RPATH	Mark Abraham	10/16/2019 10:28 AM	2020-beta3
2715	GROMACS	Feature	New	Normal	Avoid requesting the user to recompile gromacs for Intel OpenCL support		10/31/2018 12:16 PM	2020
2713	GROMACS	Feature	New	Normal	Constant offset for external electric fields		10/28/2018 12:57 AM	
2710	GROMACS	Feature	New	Normal	Separate dvdI for each molecule (of couple-moltype) when running FEP		10/26/2018 10:24 AM	2020
2707	GROMACS	Bug	New	Normal	Installed OpenCL files include clh file from gpu_utils directory		10/30/2018 04:02 AM	
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
2696	GROMACS	Task	In Progress	Normal	ensure PME queue is flushed	Szilárd Páll	12/31/2018 11:21 AM	future
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	
2667	GROMACS	Feature	New	Normal	Suggested steps for calculating entropy in solution and binding	David van der Spoel	10/30/2018 02:06 PM	2020
2660	GROMACS	Task	New	Low	rework OpenCL nbxn kernel constants	Szilárd Páll	10/30/2018 12:10 PM	2020
2658	GROMACS	Task	New	Normal	Secondary structure assignment via DSSP as native gromacs code	Christian Blau	10/09/2018 04:51 PM	future
2657	GROMACS	Bug	New	Normal	Biphasic tutorial		09/28/2018 10:02 AM	
2650	GROMACS	Task	New	Normal	revise OpenCL stack recommendations		12/31/2018 11:19 AM	future
2649	GROMACS	Bug	New	Normal	Virial calculation necessary for correct energy calculation on GPU		12/17/2018 02:32 PM	future
2645	GROMACS	Bug	New	Normal	Security		09/28/2018 01:16 PM	
2644	GROMACS	Task	New	Normal	Replace compute_globals	Mark Abraham	09/24/2018 05:51 PM	future
2643	GROMACS	Feature	New	Low	mdp options and/or docs for anisotropic aspects of implementations		09/12/2018 02:23 PM	
2637	GROMACS	Bug	New	High	gmx solvate tears apart molecules		09/11/2018 07:43 PM	

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
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
2621	GROMACS	Task	New	Normal	Fine-Grained API to Describe Force Calculation and Neighbourhood Search	Prashanth Kanduri	08/22/2018 11:36 AM	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	
2603	GROMACS	Task	New	Normal	Add ability to properly check coordinate files during testing	Paul Bauer	10/15/2018 01:16 PM	future
2602	GROMACS	Bug	New	Low	build information gets outdated if build tree is reused		08/13/2018 09:04 PM	
2601	GROMACS	Feature	New	Normal	Free energy calculations, soft-core potential	Vytautas Gapsys	03/05/2019 01:44 AM	future
2600	GROMACS	Bug	New	High	coul-lambdas turns off all coulombic interactions in system instead of the molecule specified in the couple-moltype		08/07/2018 06:50 PM	
2598	GROMACS	Bug	New	Normal	Tools using read_next_x cannot read TNG files with sanitizers		10/15/2018 01:16 PM	future
2596	GROMACS	Feature	New	Normal	Constant potential method	Benson Muite	05/10/2019 09:54 AM	
2595	GROMACS	Task	New	Normal	Reusable Utilities for Schedules	Prashanth Kanduri	02/22/2019 03:48 PM	future
2594	GROMACS	Feature	New	Normal	Multi-level GMX API	Prashanth Kanduri	02/22/2019 03:48 PM	future
2590	GROMACS	Task	New	Normal	Essential Dynamics as module providing forces	Christian Blau	08/22/2018 05:03 PM	future
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	
2582	GROMACS	Bug	Blocked, need info	Normal	Compilation issues with CUDA V9.1.85 and both gcc5 and gcc6	Szilárd Páll	07/23/2018 07:46 PM	

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
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	
2574	GROMACS	Feature	New	Normal	iForceSchedule Abstraction	Prashanth Kanduri	03/29/2019 05:20 PM	future
2573	GROMACS	Bug	New	High	Different mdp files describing the same change yield different free energy on the same trajectory		07/19/2018 06:52 PM	
2570	GROMACS	Feature	New	Normal	Better string formatting and printing		05/02/2019 12:20 PM	
2568	GROMACS	Bug	New	Low	gmx editconf -rotate does not rotate the box		07/10/2018 10:27 AM	future
2567	GROMACS	Bug	New	Normal	make check fails at test 23 SIMD errors		07/10/2018 09:35 AM	
2564	GROMACS	Bug	New	Normal	Result Summary Different For Jobs With Different Numbers of Nodes		07/05/2018 02:39 PM	
2563	GROMACS	Bug	New	Normal	Windows 7 Compilation with GPU support		07/02/2018 09:58 AM	
2556	GROMACS	Feature	New	Normal	make default selections suitable for DNA and RNA	Mark Abraham	06/20/2018 01:48 PM	
2555	GROMACS	Bug	New	Low	building GROMACS 2018.2		07/03/2018 11:41 PM	
2553	GROMACS	Bug	Accepted	Normal	Incorrect COM velocity correction with frozen atoms	Berk Hess	12/03/2018 01:15 PM	2020
2547	GROMACS	Feature	New	Low	Add option of averaging and obtaining error bars for AWH PMFs	Viveca Lindahl	06/06/2018 11:31 AM	future
2546	GROMACS	Task	New	Normal	Add more assertions to AWH code	Viveca Lindahl	06/06/2018 11:20 AM	future
2545	GROMACS	Feature	New	Normal	Should grompp fix periodicity of input files?	David van der Spoel	10/03/2018 11:32 PM	future
2544	GROMACS	Bug	New	Normal	gmx rmsf does not fix periodicity in reference structure	David van der Spoel	08/21/2018 10:36 AM	future
2538	GROMACS	Task	New	Normal	organize more of the PME GPU code along task-specific lines	Mark Abraham	05/31/2018 05:41 PM	
2537	GROMACS	Task	New	Normal	Simplify PME solve reduction	Aleksei lupinov	10/30/2018 12:08 PM	2020
2535	GROMACS	Task	New	Normal	consider compiling opencl fft kernels once		05/31/2018 01:33 PM	
2532	GROMACS	Task	New	Normal	enable queue priorities in OpenCL		05/29/2018 02:29 PM	
2531	GROMACS	Task	New	Low	Consider optimizing tabulated data access on GPU		07/30/2018 12:31 PM	
2530	GROMACS	Task	New	Normal	consider using CUDA Driver API		09/23/2018 11:47 PM	future
2528	GROMACS	Task	New	Normal	PME GPU tuning		12/31/2018 11:18 AM	future

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
2527	GROMACS	Task	New	Normal	Rename GpuEventSynchronizer to something more fitting (after merge in PME OpenCL)		10/30/2018 04:06 AM	future
2526	GROMACS	Bug	New	Normal	Bug of gmx hbond		05/30/2018 03:12 PM	
2524	GROMACS	Task	New	Normal	struct alignment/packing for OpenCL host & device code		10/30/2018 12:06 PM	2020
2522	GROMACS	Task	New	Normal	OpenCL context duplication		10/30/2018 12:07 PM	2020
2521	GROMACS	Task	New	Normal	Implement alternating PME/NB wait for OpenCL		10/15/2018 12:39 PM	
2520	GROMACS	Task	New	Normal	Treat OpenCL kernel width more diligently		05/24/2018 06:21 PM	
2519	GROMACS	Task	New	High	Improve/remove PME OpenCL kernel barriers		02/15/2019 06:34 PM	
2518	GROMACS	Task	New	Normal	redesign task-assignment code for OpenCL		12/28/2018 12:38 PM	2020
2516	GROMACS	Task	New	Low	Support PME OpenCL execution width < 16	Aleksei lupinov	06/05/2019 05:32 PM	
2514	GROMACS	Task	New	Normal	PME OpenCL reductions with intrinsics		05/31/2018 12:27 AM	future
2513	GROMACS	Bug	Feedback wanted	Normal	ref_t and temperature incorrect with coulomb-type = user	Yu Du	05/31/2018 04:05 PM	
2501	GROMACS	Task	New	Normal	Documentation section on log file contents	Kevin Boyd	10/03/2018 09:48 PM	future
2498	GROMACS	Task	New	Normal	OpenCL memory pinning/mapping		10/30/2018 12:07 PM	2020
2496	GROMACS	Task	New	Low	find system xdr properly		05/02/2018 02:19 PM	
2495	GROMACS	Task	New	Normal	replace -noconfout with mdp option	Mark Abraham	10/12/2018 10:34 PM	2020
2492	GROMACS	Task	New	Normal	implement force calculation via ForceProviders containing collections of IForceProvider	Mark Abraham	09/19/2018 03:13 PM	future
2491	GROMACS	Feature	New	Low	Allow constant bias AWH simulations	Viveca Lindahl	06/05/2018 10:38 PM	future
2490	GROMACS	Task	New	Normal	evaluate two-step communicators	Szilárd Páll	10/03/2018 09:47 PM	future
2488	GROMACS	Task	New	Normal	use MPI non-blocking collectives to overlap pull comm		04/25/2018 04:19 PM	
2483	GROMACS	Bug	New	Low	gmx dump writes mdp files that can not be parsed by grompp	Paul Bauer	10/08/2018 10:50 AM	future
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
2480	GROMACS	Bug	New	Normal	pdb2gmx does not protonate correctly for united-atom Gromos	Mark Abraham	12/17/2018 01:27 PM	2020
2478	GROMACS	Task	New	Low	avoid use of getenv in static initialization		04/13/2018 11:57 AM	
2475	GROMACS	Task	New	Normal	make OpenCL 1st class-citizen in the build system		10/30/2018 12:01 PM	2020
2473	GROMACS	Bug	New	Normal	mdrun sometimes stalls due to large coordinates with no constraints		04/04/2018 10:15 PM	
2469	GROMACS	Task	New	Normal	implement GPU timer reduction for reporting		03/27/2018 05:08 PM	

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
2468	GROMACS	Bug	New	Low	incorrect GPU timing reported with OpenCL and domain decomposition		12/17/2018 01:28 PM	future
2464	GROMACS	Task	New	Normal	GPU performance goals overview		03/26/2018 10:42 AM	
2463	GROMACS	Task	New	Low	PME GPU decomposition		03/26/2018 10:42 AM	
2462	GROMACS	Task	New	Normal	consider adding STL misuse tests		03/23/2018 01:23 AM	
2460	GROMACS	Bug	New	Normal	Allow inclusion of user libraries through CMake cache variables		03/28/2018 08:47 PM	
2456	GROMACS	Task	New	Normal	Add a pull module external potential tests		03/15/2018 03:02 PM	
2453	GROMACS	Task	Resolved	High	PME OpenCL porting effort	Aleksei lupinov	06/05/2019 05:32 PM	2020
2452	GROMACS	Task	In Progress	Normal	Reduce data dependencies in mdrun algorithms	Berk Hess	03/14/2018 08:47 PM	
2451	GROMACS	Feature	Resolved	Normal	Linear virtual sites with fixed distance	David van der Spoel	09/16/2019 01:15 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	
2442	GROMACS	Task	New	Normal	Port gmx saxs and gmx sans to c++	Joe Jordan	06/28/2018 10:06 PM	future
2435	GROMACS	Task	New	Normal	identify and note about/tune task offload in GPU-bound runs		03/02/2018 04:08 PM	
2429	GROMACS	Feature	New	Normal	Add option of periodic chain topology to pdb2gmx		03/10/2018 01:01 PM	
2428	GROMACS	Feature	New	Normal	Add way of selecting interactive arguments of pdb2gmx by string rather than an index		02/27/2018 06:28 PM	
2427	GROMACS	Bug	New	Normal	gmx select gives syntax error for selection involving evaluating simple arithmetic expression		02/27/2018 05:15 PM	
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
2425	GROMACS	Task	New	Normal	testing multisim with multiple ranks per simulation	Mark Abraham	11/29/2018 11:20 AM	2020
2423	GROMACS	Task	New	Normal	modernize constraints code	Mark Abraham	09/19/2018 03:01 PM	future
2422	GROMACS	Task	New	Normal	write C kernel for tables in Verlet scheme		02/26/2018 01:38 PM	
2412	GROMACS	Task	New	Normal	attempt to do better FFTW planning		03/15/2018 05:01 PM	
2402	GROMACS	Task	New	Normal	PME kernels general performance improvements		03/26/2018 10:41 AM	future
2396	GROMACS	Task	New	Normal	Refactor trajectoryanalysis module to allow handling of trajectory frame manipulation	Paul Bauer	10/08/2018 07:29 PM	2020
2395	GROMACS	Task	In Progress	Normal	break up commrec	Mark Abraham	09/19/2018 03:13 PM	2020
2393	GROMACS	Bug	New	Normal	incorrect error message with omitted command line flag before its argument		01/24/2018 11:24 PM	

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
2391	GROMACS	Task	Accepted	Normal	re-enable TPI test	Berk Hess	01/09/2019 05:17 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
2383	GROMACS	Task	New	Normal	Add JSON interface to write and read files	Paul Bauer	01/16/2018 02:01 PM	future
2382	GROMACS	Task	New	Normal	Simplify Doxygen guidelines		01/13/2018 12:40 AM	
2380	GROMACS	Bug	New	Low	cycle counter issues with separate PME rank + GPUs		01/16/2018 10:21 PM	
2379	GROMACS	Task	New	Normal	check leftover FIXMEs in r2018	Szilárd Páll	12/31/2018 11:16 AM	future
2376	GROMACS	Task	New	Normal	max_mpi_ranks has wrong name		02/10/2018 11:03 AM	
2375	GROMACS	Task	New	Normal	Clarify execution phases for MD simulation		04/30/2019 12:59 PM	
2373	GROMACS	Bug	New	Low	gmx -nice can't work		01/04/2018 11:17 AM	
2371	GROMACS	Task	New	Normal	mtop searching needs reconsideration		01/04/2018 11:54 AM	future
2368	GROMACS	Task	In Progress	Normal	update implementation of gmx msd	Kevin Boyd	11/03/2018 07:43 PM	future
2367	GROMACS	Task	New	Normal	construct pbc_simd less often		09/24/2018 11:02 PM	future
2360	GROMACS	Bug	New	Low	error at counter reset with PME-only rank		01/05/2018 12:43 PM	future
2354	GROMACS	Feature	New	Normal	develop configuration file support for control of task layout		09/19/2018 03:01 PM	future
2353	GROMACS	Task	New	Normal	improve on relative tolerance for constructing tables		10/30/2018 04:17 AM	2020
2351	GROMACS	Task	New	Normal	Avoid the SIMD module depending on non-trivial parts of Gromacs		12/14/2017 02:47 AM	future
2341	GROMACS	Task	New	Low	assess the state of building and using GROMACS on Windows		07/29/2019 11:09 PM	future
2310	GROMACS	Feature	Accepted	Low	Let mdrun dump coordinates with non-finite energy		10/03/2018 09:47 PM	future
2304	GROMACS	Task	New	Normal	Document and propose tracking mdrun heuristics		10/03/2018 09:39 PM	future
2294	GROMACS	Task	New	Normal	Require identical hardware on nodes on parallel runs		11/19/2017 08:54 PM	
2289	GROMACS	Feature	New	Normal	gmx spatial add ability to perform over multiple reference structures		11/08/2017 12:31 AM	
2288	GROMACS	Feature	Accepted	Low	gmx msd doesn't optimally handle missing input trajectory frames		11/10/2017 11:03 AM	
2283	GROMACS	Feature	New	Normal	Force distribution analysis	Bernd Doser	10/27/2017 11:44 AM	
2282	GROMACS	Feature	New	Normal	Density map toolset	Christian Blau	03/21/2019 06:08 PM	future
2281	GROMACS	Task	In Progress	Normal	Represent data on regularly spaced N-dimensional grids.	Christian Blau	08/06/2019 08:48 AM	2020
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	

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
2238	GROMACS	Task	In Progress	Normal	GPU emulation mode support for rolling pruning missing	Berk Hess	12/21/2017 03:21 PM	
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	
2229	GROMACS	Feature	New	High	Full Object Oriented Modularization of GROMACS MDRUN Codebase	Mark Abraham	08/22/2018 05:03 PM	future
2226	GROMACS	Feature	New	Normal	Harmonise commands for exit in make_ndx and distance		08/04/2017 12:24 PM	
2224	GROMACS	Feature	New	Normal	Proposed feature: conditional stop	Vedran Miletic	09/19/2018 03:06 PM	2020
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	
2216	GROMACS	Task	New	Normal	GROMACS SIMD acceleration: generation 3	Erik Lindahl	07/17/2017 06:57 PM	future
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	
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
2186	GROMACS	Feature	New	Low	Potential change for logical improvements: move control of constraints purely to the .mdp	Michael Shirts	11/27/2018 11:27 AM	future
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	
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
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	
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	

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
2137	GROMACS	Feature	New	Normal	Preliminary refactoring of constraints and update machinery.	Michael Shirts	03/11/2017 08:32 AM	future
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	
2097	GROMACS	Feature	New	Low	Move output of dhdl file entirely to edr, rather than having a separate text dhdl file		01/05/2017 05:21 PM	future
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
2090	GROMACS	Feature	New	Normal	redirecting stdout or stderr for testing	Mark Abraham	12/15/2016 03:15 AM	
2089	GROMACS	Task	New	Normal	Encourage code review		01/10/2017 12:03 AM	
2084	GROMACS	Task	New	Low	MPI and stderr/log output		11/28/2016 06:37 PM	
2080	GROMACS	Feature	New	Normal	add grompp warning for suitability for domain decomposition		11/23/2016 03:03 PM	
2071	GROMACS	Task	In Progress	High	Low accuracy default settings yield incorrect liquid densities	Berk Hess	01/05/2018 03:32 PM	
2070	GROMACS	Feature	In Progress	Normal	Physical validation testing	Michael Shirts	10/12/2018 10:36 PM	2020
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	
2054	GROMACS	Feature	Accepted	High	PME on GPU	Aleksei lupinov	10/03/2019 09:41 PM	2020
2053	GROMACS	Task	New	Normal	refine notation in GPU code		09/04/2019 01:47 PM	2020

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