

Issues

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
3446	GROMACS	Task	New	Normal	apply maintainability updates across all GPU kernels	Jonathan Vincent	03/19/2020 03:31 PM	
3445	GROMACS	Task	New	Normal	create heuristic for c_skipNeutralAtoms	Jonathan Vincent	03/17/2020 12:12 PM	
3437	GROMACS	Task	New	Normal	Use builders to prepare modules	Pascal Merz	03/11/2020 07:05 AM	2021-infrastructure-stable
3422	GROMACS	Task	Resolved	Normal	Implement modular checkpointing for modular simulator	Pascal Merz	09/16/2020 09:45 AM	2021-infrastructure-stable
3421	GROMACS	Task	New	Normal	Implement client system for global reduction	Pascal Merz	03/11/2020 03:31 PM	2021-infrastructure-stable
3420	GROMACS	Task	New	Normal	Unify force and shellfc elements for modular simulator	Pascal Merz	03/10/2020 09:50 PM	2021-infrastructure-stable
3419	GROMACS	Task	New	Normal	Reduce / remove use of legacy t_state objects throughout modular simulator	Pascal Merz	03/10/2020 10:24 PM	2021-infrastructure-stable
3418	GROMACS	Task	New	Normal	Infrastructure improvements for modular simulator	Pascal Merz	03/10/2020 10:24 PM	2021-infrastructure-stable
3416	GROMACS	Task	New	Normal	Port post-submit matrix to Gitlab CI	Joe Jordan	03/16/2020 05:50 PM	2021-refactoring
3415	GROMACS	Task	New	Normal	Port Pre-submit matrix to Gitlab CI	Szilárd Páll	03/23/2020 10:09 AM	2021-refactoring
3392	GROMACS	Task	New	Low	Unify box correction for modular simulator	Pascal Merz	03/11/2020 05:20 PM	2021-infrastructure-stable
3382	GROMACS	Task	Accepted	Normal	Split up t_inputrec		02/17/2020 05:28 PM	
3370	GROMACS	Task	New	High	Further improvements to GPU Buffer Ops and Comms		03/04/2020 01:38 PM	
3366	GROMACS	Task	New	Normal	Enforce compability of MdModules		02/28/2020 11:20 AM	
3365	GROMACS	Task	New	Low	consider making GPU bonded work independent from nonbonded		03/01/2020 01:11 PM	
3361	GROMACS	Task	New	Normal	Gitlab source archive contains files from build directory	Paul Bauer	02/25/2020 10:13 AM	2020.2
3360	GROMACS	Task	New	Normal	investigate the future of DD dynamic load balancing with GPU offload		01/29/2020 11:23 AM	
3357	GROMACS	Task	New	Normal	Make sure "colvars" interoperates stably and smoothly with gromacs		03/04/2020 11:25 AM	
3356	GROMACS	Task	New	Normal	Expose setting of random seed to API		01/29/2020 06:16 PM	2021
3353	GROMACS	Task	New	Normal	Document gmx densmap output		01/23/2020 12:52 PM	
3348	GROMACS	Task	New	Normal	GPU LINCS and SETTLE: unify virial reduction	Artem Zhmurov	01/23/2020 11:58 AM	2021-infrastructure-stable
3346	GROMACS	Task	New	Normal	GPU SETTLE: Use the same parameters and parameters initialization in GPU and CPU versions of SETTLE.	Artem Zhmurov	01/23/2020 11:58 AM	2021-infrastructure-stable
3345	GROMACS	Task	New	Normal	GPU update-constraints: Reconsider the naming of coordinates buffer in constraints.	Artem Zhmurov	01/23/2020 11:57 AM	2021-infrastructure-stable
3344	GROMACS	Task	New	Normal	GPU update-constraints: Better virial reduction.	Artem Zhmurov	01/23/2020 11:57 AM	2021-infrastructure-stable
3343	GROMACS	Task	New	Normal	GPU SETTLE: Use different ordering for matrices.	Artem Zhmurov	01/23/2020 11:57 AM	2021-infrastructure-stable

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3342	GROMACS	Task	New	Normal	GPU SETTLE: Read only one index per water molecule.	Artem Zhmurov	01/23/2020 11:56 AM	2021-infrastructure-stable
3341	GROMACS	Task	New	Normal	GPU LINCS: Use analytical solution for the matrix A inversion.	Artem Zhmurov	01/23/2020 11:56 AM	2021-infrastructure-stable
3340	GROMACS	Task	New	Normal	GPU LINCS: Move more data to local/shared memory	Artem Zhmurov	01/23/2020 11:56 AM	2021-infrastructure-stable
3339	GROMACS	Task	New	Normal	GPU LINCS: Warp-level synchronization for coupled constraints	Artem Zhmurov	01/23/2020 11:55 AM	2021-infrastructure-stable
3338	GROMACS	Task	New	Normal	GPU update-constraints: Do not save intermediate coordinates if there is no constraints	Artem Zhmurov	01/23/2020 11:55 AM	2021-infrastructure-stable
3337	GROMACS	Task	New	Normal	GPU update-constraints: Merge Leap-Frog, LINCS and SETTLE kernels.	Artem Zhmurov	01/23/2020 11:55 AM	2021-infrastructure-stable
3331	GROMACS	Task	New	Low	Run physical validation tests in Gitlab	Paul Bauer	02/27/2020 11:09 PM	future
3330	GROMACS	Task	New	Normal	Compile list of codepaths for testing task assignment		01/22/2020 10:03 AM	2021-refactoring
3329	GROMACS	Task	New	Normal	Extend energy comparison testing framework		01/22/2020 09:51 AM	2021-refactoring
3327	GROMACS	Task	New	Normal	Refactor workload flags		01/22/2020 09:45 AM	2021-refactoring
3326	GROMACS	Task	New	Normal	Allow changing task assignment		01/22/2020 09:44 AM	2021-refactoring
3325	GROMACS	Task	New	Normal	Allow complete re-initialization of a simulation		01/29/2020 05:13 PM	2021-refactoring
3324	GROMACS	Task	New	Normal	Rework CMake handling of GPU code		01/22/2020 09:52 AM	2021-refactoring
3323	GROMACS	Task	In Progress	Normal	Rework the StatePropagatorDataGpu	Artem Zhmurov	01/22/2020 09:50 AM	2021-refactoring
3322	GROMACS	Task	Accepted	Normal	Add reallocate(...) function that does not care about the contents of the buffer	Artem Zhmurov	01/22/2020 09:50 AM	2021-refactoring
3321	GROMACS	Task	Accepted	Normal	Add D2D wrapper	Artem Zhmurov	01/22/2020 09:50 AM	2021-refactoring
3320	GROMACS	Task	In Progress	Normal	Remove duplicating D2H/H2D wrappers in NBNXM	Artem Zhmurov	01/22/2020 09:50 AM	2021-refactoring
3319	GROMACS	Task	In Progress	Normal	Use DeviceBuffer instead of native GPU types in NBNXM	Artem Zhmurov	01/22/2020 09:49 AM	2021-refactoring
3317	GROMACS	Task	Resolved	Normal	Improve testing of the GPU code	Artem Zhmurov	10/06/2020 12:15 PM	2021-refactoring
3316	GROMACS	Task	Accepted	Normal	Context and Stream manager	Artem Zhmurov	01/22/2020 09:49 AM	2021-refactoring
3315	GROMACS	Task	Resolved	Normal	Platform agnostic DeviceContext	Artem Zhmurov	03/11/2020 04:15 PM	2021-refactoring
3314	GROMACS	Task	Resolved	Normal	Platform agnostic DeviceStream	Artem Zhmurov	03/20/2020 09:55 AM	2021-refactoring
3312	GROMACS	Task	In Progress	Normal	Data type for coordinates, xyzq data, LJ parameters data to use for GPU buffers	Artem Zhmurov	03/20/2020 09:54 AM	2021-refactoring

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3308	GROMACS	Task	New	Normal	GPU update-constraints: Cycle counting for GPU launches		01/23/2020 11:54 AM	2021-infrastructure-stable
3306	GROMACS	Task	New	Normal	Document gmx dos tool more clearly	Christian Blau	01/20/2020 02:31 PM	future
3300	GROMACS	Task	New	Normal	Abandon docs/OpenCLTODOList.txt?		01/15/2020 02:46 PM	
3297	GROMACS	Task	Resolved	Normal	Require gcc > 5		04/30/2020 11:00 AM	2021-infrastructure-stable
3290	GROMACS	Task	Resolved	Normal	Require CMake >= 3.12		04/14/2020 02:45 PM	2021-refactoring
3289	GROMACS	Task	New	Normal	Distinguish identifying and non-identifying inputs to API operations.	Eric Irrgang	01/10/2020 11:30 AM	
3287	GROMACS	Task	New	Normal	Deprecate make_ndx, use select instead		01/23/2020 01:16 PM	
3279	GROMACS	Task	New	Low	Provide more advice for building client software		03/02/2020 11:54 AM	
3275	GROMACS	Task	New	Normal	Document Gitlab CI instead of Jenkins and releng	Paul Bauer	03/09/2020 05:55 PM	2021-infrastructure-stable
3272	GROMACS	Task	New	Normal	Port complete CI testing to Gitlab	Paul Bauer	02/27/2020 11:04 AM	2021-infrastructure-stable
3271	GROMACS	Task	Resolved	Normal	Adopt PEP-518 for Python package build system configuration.		04/09/2020 10:15 PM	2021-infrastructure-stable
3268	GROMACS	Task	New	Normal	add more Intel driver recommendations		12/26/2019 04:39 PM	
3267	GROMACS	Task	New	Normal	Document tools		12/26/2019 03:20 PM	future
3264	GROMACS	Task	New	Normal	Break up MdrunMpiTests	Paul Bauer	12/23/2019 11:44 AM	2021-infrastructure-stable
3262	GROMACS	Task	New	High	Trjconv - dimer protein-ligand		12/20/2019 09:26 PM	
3260	GROMACS	Task	New	Low	keep up to with mdspan reference implementation	Christian Blau	12/20/2019 01:16 PM	2021-infrastructure-stable
3258	GROMACS	Task	New	Normal	GPU update-constraints: Enable free energy perturbation	Artem Zhmurov	01/23/2020 11:54 AM	2021-infrastructure-stable
3256	GROMACS	Task	New	Normal	Remove -nsteps option from mdrun		12/19/2019 12:12 PM	
3255	GROMACS	Task	New	Normal	Move benchmarking options from mdrun to a dedicated tool		12/19/2019 01:21 PM	
3254	GROMACS	Task	New	Normal	Remove support for generation of virtual sites to replace aromatic rings in standard residues		12/19/2019 12:13 PM	
3252	GROMACS	Task	New	Normal	Remove support for 32 bit architectures		03/01/2020 02:05 PM	
3236	GROMACS	Task	New	Normal	GPU update-constraints: Pulling support	Artem Zhmurov	01/23/2020 11:53 AM	2021-infrastructure-stable
3235	GROMACS	Task	New	Normal	Run mdrun-test in parallel and make sure they tests test critical quantities like energy conservation	Christian Blau	12/12/2019 03:46 PM	2021-infrastructure-stable
3229	GROMACS	Task	New	Normal	Move checkpointing to the beginning of the MD step		01/16/2020 04:31 PM	2021-infrastructure-stable
3224	GROMACS	Task	New	Normal	add regression test case large enough to miscalculated GPU grid launch cases		12/20/2019 01:18 PM	2021
3220	GROMACS	Task	New	Normal	change rolling pruning scheduling with GPU update		02/25/2020 03:41 PM	2021-infrastructure-stable
3216	GROMACS	Task	New	Normal	improve CPU force reductions	Szilárd Páll	12/04/2019 09:24 PM	
3212	GROMACS	Task	New	Normal	Update regression tests for new kernel flavours		11/21/2019 11:50 AM	
3203	GROMACS	Task	Accepted	Normal	Tools should check that input is valid when first using it	Paul Bauer	12/03/2019 05:26 PM	2021-infrastructure-stable

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3201	GROMACS	Task	In Progress	Normal	Convert mdp parameters to key value tree		11/06/2019 06:06 PM	
3194	GROMACS	Task	New	Normal	consider passing GPU dependency list to both dependency producers and consumers		11/01/2019 07:10 PM	
3189	GROMACS	Task	In Progress	High	implement heuristics for switching between different spread/gather kernel layouts	Jonathan Vincent	01/29/2020 04:18 PM	2021-infrastructure-stable
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		12/20/2019 08:32 AM	2021-infrastructure-stable
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	02/14/2020 12:45 PM	2021-infrastructure-stable
3174	GROMACS	Task	Feedback wanted	Low	Proposed gmxapi syntax update: "input" and "output" key word arguments -> "inputs" and "outputs"	Eric Irrgang	10/23/2019 06:34 PM	
3171	GROMACS	Task	New	Normal	schedule CPU H2D force contribution in separate stream		12/20/2019 08:33 AM	2021-infrastructure-stable
3162	GROMACS	Task	New	Normal	Add virtual site support to GPU version of update-constraints.	Artem Zhmurov	01/23/2020 11:52 AM	2021-infrastructure-stable
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	Resolved	Low	Update use of Python subprocess for >=3.5		04/09/2020 10:15 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
3145	GROMACS	Task	New	Normal	gmxapi.mdrun needs improved (and public) interface for attaching an MD extension.	Eric Irrgang	01/16/2020 04:31 PM	2021-refactoring
3143	GROMACS	Task	New	Normal	move the non-force accumulation/accounting tasks out of the GPU wait functions	Szilárd Páll	12/27/2019 04:16 PM	2021
3139	GROMACS	Task	New	Normal	gmxapi Futures should be subscribable	Eric Irrgang	10/15/2019 03:56 PM	
3133	GROMACS	Task	In Progress	Normal	Cookiecutter for sample_restraint	Eric Irrgang	12/10/2019 01:59 PM	2021-infrastructure-stable
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	12/20/2019 08:20 AM	2021-infrastructure-stable
3130	GROMACS	Task	New	Normal	Interim handling of gmxapi data references.	Eric Irrgang	12/11/2019 11:26 AM	2021-infrastructure-stable
3123	GROMACS	Task	New	Normal	address sanitizer coverage of parallelization code-paths		10/05/2019 12:32 AM	
3119	GROMACS	Task	New	Normal	clang-tidy coverage of parallelization codepaths		12/27/2019 04:20 PM	2021
3105	GROMACS	Task	New	Normal	implement GPU PME/PP comm cycle counting		12/27/2019 04:20 PM	2021
3104	GROMACS	Task	New	Normal	implement GPU DD cycle counting		12/27/2019 04:21 PM	2021

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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		02/14/2020 11:35 AM	2021-infrastructure-stable
3082	GROMACS	Task	New	High	move launch/synchronization points to clarify task dependencies		12/27/2019 04:21 PM	2021
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	01/17/2020 02:40 PM	2021-infrastructure-stable
3072	GROMACS	Task	New	Normal	Use gm::index for indexing instead of int	Christian Blau	09/03/2019 04:23 PM	2021-infrastructure-stable
3064	GROMACS	Task	New	Normal	add test for perturbed bonded forces		12/27/2019 04:22 PM	2021
3062	GROMACS	Task	New	Normal	add twin cut-off mdrun test		12/27/2019 04:22 PM	2021
3057	GROMACS	Task	New	Normal	re-enable fusion on Power8/9	Szilárd Páll	12/27/2019 04:22 PM	2021
3047	GROMACS	Task	Feedback wanted	Normal	Set required versions for GROMACS 2021		02/20/2020 11:42 AM	
3041	GROMACS	Task	Resolved	Normal	Remove workaround for gcc bug 58265		06/19/2020 04:45 PM	
3040	GROMACS	Task	New	Normal	Refactor Restraint module		07/18/2019 03:59 PM	
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		01/16/2020 04:50 PM	2021-refactoring
3031	GROMACS	Task	New	Normal	evaluate the impact of particle order on PME		12/27/2019 04:29 PM	2021
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 gm_fatal		09/06/2019 02:34 PM	2021-infrastructure-stable
3014	GROMACS	Task	In Progress	Normal	gmapi example Python scripts		01/03/2020 11:00 AM	2021-infrastructure-stable
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		12/20/2019 08:25 AM	2021-infrastructure-stable
3008	GROMACS	Task	New	Normal	verify block size choice of CUDA bonded kernel		12/27/2019 04:30 PM	2021
3005	GROMACS	Task	New	Normal	Move logging in gm 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		12/27/2019 04:30 PM	2021
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	Resolved	Normal	Update Python detection		04/23/2020 04:45 PM	2021-infrastructure-stable

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2997	GROMACS	Task	New	Normal	improve performance of alchemical free energy calculations		12/27/2019 04:31 PM	2021
2992	GROMACS	Task	New	Normal	Split hw_opt in const user options and dynamic settings		12/27/2019 04:31 PM	future
2988	GROMACS	Task	In Progress	Low	clean up and refactor code to modern standards		12/27/2019 04:37 PM	future
2983	GROMACS	Task	New	Normal	better suited data-types for bonded GPU kernels		07/11/2019 04:32 PM	
2976	GROMACS	Task	New	Normal	Basic math for Multidimensional arrays		12/27/2019 04:37 PM	2021
2965	GROMACS	Task	In Progress	Normal	Performance of GPU direct communications		02/14/2020 12:38 PM	2021
2947	GROMACS	Task	Accepted	Normal	make an end to end test for membed		09/24/2019 03:22 PM	future
2936	GROMACS	Task	New	Normal	introduce check that CPU-GPU transfers/assignments are made between compatible types		02/05/2020 03:57 PM	2021
2933	GROMACS	Task	New	Normal	Convert walls to a ForceProvider		04/25/2019 02:43 PM	
2925	GROMACS	Task	New	Normal	BasicVector addition operator yields unexpected result when adding scalar	Christian Blau	12/17/2019 10:04 AM	2021-infrastructure-stable
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
2909	GROMACS	Task	New	Normal	consider implementing mechanisms to ensure pair lists are not used past their max lifetime		04/03/2019 05:14 PM	
2908	GROMACS	Task	New	Normal	Renaming things in nbxnm	Berk Hess	03/28/2019 10:10 AM	
2905	GROMACS	Task	New	Normal	Add a Jenkins configuration with std library assert		08/24/2019 05:22 PM	
2898	GROMACS	Task	New	Low	Naming common variables		03/26/2019 11:46 PM	
2889	GROMACS	Task	New	Normal	update grompp warnings for brevity, usefulness and actionability	Mark Abraham	12/27/2019 04:38 PM	future
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	12/20/2019 01:22 PM	2021
2875	GROMACS	Task	Accepted	Normal	SIMD version of the free-energy kernel	Berk Hess	12/02/2019 01:44 PM	2021-infrastructure-stable
2874	GROMACS	Task	New	Normal	Refactor Gromacs (cluster) neighborlist into separate module	Erik Lindahl	02/28/2019 11:36 AM	
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	
2859	GROMACS	Task	Resolved	Normal	Change ArrayRef iterator type from pointer to std::iterator		06/26/2020 06:15 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		01/10/2020 12:06 PM	
2850	GROMACS	Task	In Progress	Normal	assess Raptor Talos for testing	Szilárd Páll	02/12/2019 01:14 PM	
2839	GROMACS	Task	New	Normal	make module and file naming consistent		01/16/2020 05:11 PM	2021

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2835	GROMACS	Task	New	Normal	Matrix class constraint to upper or lower triangle		02/07/2019 02:44 PM	
2834	GROMACS	Task	In Progress	Normal	C++ matrix classes	Christian Blau	12/29/2019 10:32 AM	2021
2833	GROMACS	Task	New	Normal	Update topology datastructures	Paul Bauer	12/02/2019 01:43 PM	2021-infrastructure-stable
2822	GROMACS	Task	Accepted	Normal	Make nbxn a module	Berk Hess	12/18/2019 10:49 AM	future
2818	GROMACS	Task	In Progress	Normal	bonded GPU kernel fusion	Magnus Lundborg	07/03/2019 09:01 PM	
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		12/02/2019 01:44 PM	2021-infrastructure-stable
2792	GROMACS	Task	New	High	Improvement of PME gather and spread CUDA kernels		03/18/2020 03:57 PM	
2787	GROMACS	Task	New	Normal	allow passing flags to allocateDeviceBuffer		12/03/2018 01:54 PM	
2773	GROMACS	Task	New	Normal	improve GPU error handling and make such handling uniform across modules		12/20/2019 01:09 PM	2021
2771	GROMACS	Task	New	Normal	Size independent Hessian for normal mode analysis		12/28/2019 10:50 AM	future
2770	GROMACS	Task	New	Normal	change branch maintenance policy		01/16/2020 05:09 PM	2021
2766	GROMACS	Task	In Progress	Normal	Improve hardware option selection	Kevin Boyd	12/20/2019 02:34 PM	2021
2764	GROMACS	Task	New	Normal	gmxapi version updates for post release-2019	Eric Irrgang	11/21/2018 12:53 PM	
2758	GROMACS	Task	New	Low	Modernize genconf		11/15/2018 07:38 AM	future
2756	GROMACS	Task	In Progress	Normal	gmxapi integration testing		01/16/2020 05:12 PM	2021-refactoring
2735	GROMACS	Task	New	Normal	Allow gmx_genrestr to write correct position restraints for molecules after the first molecule	Joe Jordan	12/11/2019 09:26 AM	future
2723	GROMACS	Task	New	Normal	Update mdrun-performance.rst to clearly express the nature of task	Joe Jordan	02/27/2020 11:07 AM	2020.2
2706	GROMACS	Task	Accepted	Normal	Rework classic QM/MM interface		12/02/2019 01:45 PM	2021-infrastructure-stable
2699	GROMACS	Task	New	Normal	Test POWER9		12/04/2019 03:29 PM	2021-infrastructure-stable
2698	GROMACS	Task	In Progress	Normal	gmxapi documentation integration		01/29/2020 03:59 PM	2021-infrastructure-stable
2697	GROMACS	Task	New	Normal	improve FFT library flavor/version reporting		12/27/2019 04:40 PM	future
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		12/27/2019 04:40 PM	2021
2686	GROMACS	Task	New	Normal	add tests for gpu bonded interactions		12/27/2019 04:40 PM	2021
2682	GROMACS	Task	New	Normal	Add MSAN configuration		10/09/2018 06:28 PM	
2675	GROMACS	Task	In Progress	Normal	bonded CUDA offload task		02/12/2020 05:54 PM	2021
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		12/20/2019 01:17 PM	future

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2670	GROMACS	Task	New	Low	remove old/backward compatibility OpenCL support from releng		10/04/2018 06:06 PM	
2660	GROMACS	Task	New	Low	rework OpenCL nbxn kernel constants	Szilárd Páll	12/28/2019 10:53 AM	future
2658	GROMACS	Task	New	Normal	Secondary structure assignment via DSSP as native gromacs code	Christian Blau	10/09/2018 04:51 PM	future
2650	GROMACS	Task	New	Normal	revise OpenCL stack recommendations		12/31/2018 11:19 AM	future
2644	GROMACS	Task	New	Normal	Replace compute_globals	Mark Abraham	09/24/2018 05:51 PM	future
2632	GROMACS	Task	New	Low	make sure cmake defines proper hwloc versionc with cross-compilation enabled		12/03/2018 01:35 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
2616	GROMACS	Task	New	Normal	Model for MD state		09/14/2018 05:12 PM	
2608	GROMACS	Task	New	Normal	Remove code duplication between OpenCL and CUDA		09/24/2018 12:47 PM	
2603	GROMACS	Task	New	Normal	Add ability to properly check coordinate files during testing	Paul Bauer	10/15/2018 01:16 PM	future
2595	GROMACS	Task	New	Normal	Reusable Utilities for Schedules	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
2546	GROMACS	Task	New	Normal	Add more assertions to AWH code	Viveca Lindahl	06/06/2018 11:20 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	12/20/2019 12:21 PM	future
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
2524	GROMACS	Task	New	Normal	struct alignment/packing for OpenCL host & device code		12/20/2019 12:20 PM	future
2522	GROMACS	Task	Resolved	Normal	OpenCL context duplication		03/11/2020 04:15 PM	future
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		12/20/2019 12:19 PM	future

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
2516	GROMACS	Task	New	Low	Support PME OpenCL execution width < 16	Aleksei lupinov	06/05/2019 05:32 PM	
2514	GROMACS	Task	New	Normal	PME OpenCL reductions with intrinsics		05/31/2018 12:27 AM	future
2501	GROMACS	Task	New	Normal	Documentation section on log file contents	Kevin Boyd	10/03/2018 09:48 PM	future
2498	GROMACS	Task	New	Normal	OpenCL memory pinning/mapping		12/20/2019 12:18 PM	future
2496	GROMACS	Task	New	Low	find system xdr properly		05/02/2018 02:19 PM	
2495	GROMACS	Task	Accepted	Normal	replace -noconfout with mdp option	Mark Abraham	12/28/2019 10:39 AM	2021
2492	GROMACS	Task	New	Normal	implement force calculation via ForceProviders containing collections of IForceProvider	Mark Abraham	09/19/2018 03:13 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	
2481	GROMACS	Task	New	Low	Update gmx report-methods to write more method information		12/02/2019 01:22 PM	2021-infrastructure-stable
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		12/20/2019 12:14 PM	2021
2469	GROMACS	Task	New	Normal	implement GPU timer reduction for reporting		03/27/2018 05:08 PM	
2464	GROMACS	Task	New	Normal	GPU performance goals overview		03/26/2018 10:42 AM	
2463	GROMACS	Task	New	Low	PME GPU decomposition		03/26/2018 10:42 AM	
2462	GROMACS	Task	New	Normal	consider adding STL misuse tests		03/23/2018 01:23 AM	
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	12/20/2019 12:18 PM	2021
2452	GROMACS	Task	In Progress	Normal	Reduce data dependencies in mdrun algorithms	Berk Hess	03/14/2018 08:47 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	
2425	GROMACS	Task	New	Normal	testing multisim with multiple ranks per simulation	Mark Abraham	12/20/2019 12:13 PM	2021
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

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
2396	GROMACS	Task	New	Normal	Refactor trajectoryanalysis module to allow handling of trajectory frame manipulation	Paul Bauer	12/02/2019 01:24 PM	2021-infrastructure-stable
2395	GROMACS	Task	In Progress	Normal	break up commrec	Mark Abraham	12/15/2019 11:51 AM	2021-infrastructure-stable
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	
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	
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
2353	GROMACS	Task	New	Normal	improve on relative tolerance for constructing tables		12/20/2019 12:12 PM	2021
2351	GROMACS	Task	New	Normal	Avoid the SIMD module depending on non-trivial parts of Gromacs		12/14/2017 02:47 AM	future
2341	GROMACS	Task	New	Low	assess the state of building and using GROMACS on Windows		07/29/2019 11:09 PM	future
2304	GROMACS	Task	New	Normal	Document and propose tracking mdrun heuristics		10/03/2018 09:39 PM	future
2294	GROMACS	Task	New	Normal	Require identical hardware on nodes on parallel runs		11/19/2017 08:54 PM	
2240	GROMACS	Task	Accepted	Low	GPU emulation mode support for PME missing		09/16/2017 10:02 PM	
2238	GROMACS	Task	In Progress	Normal	GPU emulation mode support for rolling pruning missing	Berk Hess	12/21/2017 03:21 PM	
2221	GROMACS	Task	New	Normal	Avoid preprocessor for SIMD functions		02/21/2018 01:43 PM	
2216	GROMACS	Task	New	Normal	GROMACS SIMD acceleration: generation 3	Erik Lindahl	07/17/2017 06:57 PM	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		12/29/2019 10:31 AM	2021
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	
2133	GROMACS	Task	New	Low	gmx traj needs reform		03/07/2017 02:02 PM	
2115	GROMACS	Task	New	Normal	trjconv does too many things, and combinations of them work poorly		10/02/2018 09:04 AM	
2092	GROMACS	Task	New	Normal	Tests running on GPU, and hardware assignment		12/19/2017 05:27 PM	future

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
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	
2071	GROMACS	Task	In Progress	High	Low accuracy default settings yield incorrect liquid densities	Berk Hess	01/05/2018 03:32 PM	
2069	GROMACS	Task	New	Low	Simple thread-parallelism inside routines		11/09/2016 06:06 PM	
2059	GROMACS	Task	In Progress	Normal	Separate different types of data in t_state		12/27/2019 04:42 PM	2021
2055	GROMACS	Task	New	Low	Wiki registration is broken		01/20/2017 11:31 AM	
2053	GROMACS	Task	New	Normal	refine notation in GPU code		12/20/2019 01:04 PM	2021
2048	GROMACS	Task	New	Normal	C++11: CUDA dependency on general headers		09/07/2016 10:30 PM	
2045	GROMACS	Task	New	Normal	API design and language bindings	Peter Kasson	01/29/2020 03:59 PM	
2035	GROMACS	Task	New	Normal	A common trajectory analysis data exchange format		03/15/2017 05:46 PM	future
2017	GROMACS	Task	In Progress	Normal	Modularize simulation option storage and reading from mdp files	Christian Blau	04/06/2018 06:07 PM	future
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	
1973	GROMACS	Task	New	Normal	OpenCL implementation wish list		05/27/2016 03:42 PM	
1971	GROMACS	Task	New	Normal	Removing buggy features vs. keeping workflows		01/19/2018 01:36 PM	future
1963	GROMACS	Task	New	Low	collect examples of systems where users tried to do something that performed badly	Mark Abraham	08/09/2016 07:30 AM	
1947	GROMACS	Task	New	Normal	Consider fixing corner case in TinyXML2	Mark Abraham	04/19/2016 01:40 AM	
1943	GROMACS	Task	Accepted	Low	make sure releases are submitted early for Debian Experimental	Szilárd Páll	12/20/2019 12:05 PM	2021
1937	GROMACS	Task	New	Low	stop supporting changing CUDA host compiler	Mark Abraham	10/15/2018 05:19 PM	future
1936	GROMACS	Task	New	Normal	treat default-able mdp fields as strings		04/02/2016 10:32 PM	future
1925	GROMACS	Task	In Progress	Normal	remove concept of unilateral global communication		12/29/2019 10:35 AM	2021
1907	GROMACS	Task	Accepted	Low	keeping compile- and run-time CPU/arch detection consistent		08/01/2016 10:09 PM	
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
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	
1852	GROMACS	Task	New	Normal	Remove group scheme		03/03/2020 09:03 PM	future
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	
1826	GROMACS	Task	New	Normal	investigate non-optimal results with CPU-GPU balancing on AMD	Szilárd Páll	12/20/2019 12:04 PM	future

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
1793	GROMACS	Task	New	Normal	cleanup of integration loop	Mark Abraham	10/31/2018 10:49 PM	future
1786	GROMACS	Task	New	Normal	Python style standards in developer docs	Peter Kasson	12/26/2019 03:15 PM	
1785	GROMACS	Task	New	Low	no pV term written to energy file when pressure coupling is anisotropic		07/26/2015 01:47 PM	future
1781	GROMACS	Task	Accepted	Normal	re-design benchmarking functionality	Mark Abraham	12/20/2019 12:03 PM	future
1768	GROMACS	Task	New	Normal	decide future of command-line options vs env vars		11/03/2016 05:51 PM	future
1758	GROMACS	Task	New	Normal	Verlet scheme reorganization / modularization	Mark Abraham	07/20/2015 06:33 PM	future
1745	GROMACS	Task	New	Normal	Moving to C++11 after Gromacs-5.1		06/01/2016 03:01 PM	
1729	GROMACS	Task	New	Normal	Resolve whether and how to resolve "state" variables stored in .tpr		05/13/2015 10:48 AM	future
1587	GROMACS	Task	New	Normal	improve the configurability of regression tests		12/20/2019 12:02 PM	2021
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	
1515	GROMACS	Task	New	Normal	improve g_bar output	Szilárd Páll	07/11/2016 08:10 PM	
1509	GROMACS	Task	New	Low	Reduce the distance dependence of shifted potentials for free energies if possible	Michael Shirts	07/11/2016 08:10 PM	
1505	GROMACS	Task	New	Normal	improve handling of logging	Mark Abraham	01/02/2019 06:06 PM	
1490	GROMACS	Task	New	Normal	Usage of forward declarations vs typedef vs #include	Mark Abraham	01/21/2015 10:23 AM	
1456	GROMACS	Task	New	Low	remove the use of nbat->alloc/free pointers	Szilárd Páll	06/20/2015 11:53 PM	
1411	GROMACS	Task	New	Normal	Future of thread_mpi	Mark Abraham	02/26/2018 04:56 PM	future
1373	GROMACS	Task	New	Low	Add missing nbnxn tests	Mark Abraham	06/09/2014 08:36 PM	
1323	GROMACS	Task	New	Normal	determine future of existing tools for	David van der Spoel	12/04/2018 11:53 AM	
1246	GROMACS	Task	New	Normal	expanded ensemble .tpr cannot be rerun	Michael Shirts	06/19/2015 01:56 PM	
1214	GROMACS	Task	New	Normal	Keep track of important changes for Changelog	Mark Abraham	06/26/2013 11:24 AM	
1211	GROMACS	Task	New	Low	improve use of preprocessor macros in CUDA kernels	Szilárd Páll	01/12/2015 06:42 PM	future
1170	GROMACS	Task	New	Normal	mdlib reorganization		11/17/2016 03:47 PM	future
1140	GROMACS	Task	New	Normal	Class design for passing options and data		07/11/2016 08:19 PM	
1056	GROMACS	Task	Accepted	Normal	status of fft5d_threads and fftw3_threads functionality	Mark Abraham	07/11/2016 08:21 PM	

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
1017	GROMACS	Task	New	Normal	C++ Vector/Matrix classes		07/11/2016 08:23 PM	
1010	GROMACS	Task	In Progress	Normal	Better support for multiple AnalysisData datasets	Teemu Murtola	07/11/2016 08:23 PM	
996	GROMACS	Task	New	Normal	C++ MPI Framework	Roland Schulz	07/14/2014 11:53 AM	future
988	GROMACS	Task	New	Normal	Definition of "public API"		08/28/2019 02:50 PM	future
986	GROMACS	Task	New	Normal	Handling C++ out-of-memory errors		12/24/2014 08:42 PM	future
948	GROMACS	Task	New	Normal	C++ thread synchronization primitives	Sander Pronk	07/11/2016 08:24 PM	
920	GROMACS	Task	In Progress	Normal	Add test framework for trajectory analysis modules	Teemu Murtola	07/11/2016 08:27 PM	
909	GROMACS	Task	New	Normal	Reimplement displacement calculation module		07/14/2014 11:30 AM	future
869	GROMACS	Task	In Progress	Normal	Make analysis data histogramming and multipoint data easier to use in parallel	Teemu Murtola	07/11/2016 08:28 PM	
867	GROMACS	Task	In Progress	Normal	Update Doxygen documentation for C++ code	Teemu Murtola	07/11/2016 08:28 PM	
838	GROMACS	Task	New	Normal	Improve generic error reporting routines		07/11/2016 08:29 PM	
765	GROMACS	Task	New	Normal	Improving serialization of data structures prior to communication	Mark Abraham	05/13/2014 10:04 AM	future
701	GROMACS	Task	New	Normal	Add symbol visibility macros		03/02/2019 01:46 AM	future
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
2851	Support Platforms	Task	New	Normal	uninstall redmine checklist plugin		01/30/2019 03:33 PM	
1815	Support Platforms	Task	In Progress	Normal	implement and execute plan for new releng machinery		10/15/2016 05:37 PM	
1508	Support Platforms	Task	New	Normal	Update master Jenkins build configurations		06/28/2014 03:59 AM	
1309	Support Platforms	Task	New	Normal	Jenkins verification improvements		06/01/2017 02:34 PM	
837	Support Platforms	Task	Resolved	Low	Consider subproject organization of the Gromacs project		07/14/2014 12:07 PM	
629	Support Platforms	Task	In Progress	Normal	List of users needs cleanup	Rossen Apostolov	02/21/2018 02:07 PM	
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	
3439	GROMACS	Feature	New	Normal	Optimize successive simulation segments		03/11/2020 01:42 PM	
3436	GROMACS	Feature	New	Normal	Implement AWH for modular simulator	Pascal Merz	03/11/2020 06:32 AM	2021-infrastructure-stable
3435	GROMACS	Feature	New	Normal	Implement pull for modular simulator	Pascal Merz	03/11/2020 06:31 AM	2021-infrastructure-stable
3434	GROMACS	Feature	New	Normal	Support box deformation in modular simulator	Pascal Merz	03/11/2020 12:50 AM	2021-infrastructure-stable

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
3433	GROMACS	Feature	New	Normal	Decide how to handle multisim with modular simulator	Pascal Merz	03/11/2020 06:42 AM	2021-infrastructure-stable
3432	GROMACS	Feature	New	Normal	Implement essential dynamics for modular simulator	Pascal Merz	03/11/2020 12:38 AM	2021-infrastructure-stable
3431	GROMACS	Feature	New	Normal	Implement virtual sites for modular simulator	Pascal Merz	03/11/2020 12:33 AM	2021-infrastructure-stable
3430	GROMACS	Feature	New	Normal	Implement NMR restraints for modular simulator	Pascal Merz	03/11/2020 12:28 AM	2021-infrastructure-stable
3428	GROMACS	Feature	New	Normal	Implement SIMD version of modular simulator propagators	Pascal Merz	03/11/2020 12:12 AM	2021-infrastructure-stable
3427	GROMACS	Feature	New	Normal	Support freeze groups in modular simulator	Pascal Merz	03/11/2020 12:07 AM	2021-infrastructure-stable
3426	GROMACS	Feature	New	Normal	Support acceleration in modular simulator	Pascal Merz	03/11/2020 04:09 PM	2021-infrastructure-stable
3425	GROMACS	Feature	New	Normal	Implement rerun for the modular simulator	Pascal Merz	03/10/2020 11:57 PM	2021-infrastructure-stable
3424	GROMACS	Feature	New	Normal	Implement stochastic dynamics / langevin integrator in modular simulator	Pascal Merz	03/10/2020 11:48 PM	2021-infrastructure-stable
3423	GROMACS	Feature	New	Normal	Implement additional temperature and pressure control algorithms for modular simulator	Pascal Merz	03/10/2020 11:22 PM	2021-infrastructure-stable
3417	GROMACS	Feature	New	Normal	Make modular simulator feature-complete	Pascal Merz	03/23/2020 03:57 AM	2021-infrastructure-stable
3410	GROMACS	Feature	New	Normal	Random Acceleration Molecular Dynamics (RAMD)	Bernd Doser	03/05/2020 03:22 PM	2021
3402	GROMACS	Feature	New	Normal	Clarify distinction between public API documentation and developer docs.		02/26/2020 04:16 PM	2021-infrastructure-stable
3401	GROMACS	Feature	New	Normal	Policy and procedure for installed headers (public API)		02/26/2020 04:17 PM	2021-infrastructure-stable
3395	GROMACS	Feature	Feedback wanted	Normal	Consider scripted composition of Dockerfiles		03/16/2020 12:16 PM	
3394	GROMACS	Feature	New	Normal	improve gmxapi error handling	Eric Irrgang	02/24/2020 11:45 AM	2021-infrastructure-stable
3393	GROMACS	Feature	Resolved	Normal	Allow gmxapi.commandline_operation to use STDIN	Eric Irrgang	02/25/2020 05:15 PM	2021-infrastructure-stable
3379	GROMACS	Feature	New	Normal	C++ API for simulation input and output		02/28/2020 10:38 AM	2021-infrastructure-stable
3378	GROMACS	Feature	New	Normal	genion usage without stdin (facilitates use in gmx python api)		02/13/2020 12:04 PM	
3374	GROMACS	Feature	New	Normal	SimulationInput abstraction		03/03/2020 05:32 PM	2021-refactoring
3371	GROMACS	Feature	New	Normal	Control FEP using AWH	Magnus Lundborg	02/06/2020 02:20 PM	2021
3369	GROMACS	Feature	New	Normal	Add quote about "the truth"		02/05/2020 05:08 PM	
3363	GROMACS	Feature	New	Normal	Improve FEP testing	Pascal Merz	03/01/2020 03:22 PM	2021-infrastructure-stable
3362	GROMACS	Feature	New	Normal	gmx traj: add an option to plot each component in a separate file		01/29/2020 06:18 PM	
3355	GROMACS	Feature	Accepted	Normal	New PME parallel (GPU) scheme	Jonathan Vincent	02/12/2020 11:58 AM	
3352	GROMACS	Feature	New	Normal	GPU update-constraints feature support	Artem Zhmurov	01/23/2020 11:59 AM	2021
3351	GROMACS	Feature	New	Normal	GPU update-constraints code organization and integration	Artem Zhmurov	01/23/2020 11:59 AM	2021

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
3350	GROMACS	Feature	New	Normal	GPU update-constraints performance	Artem Zhmurov	01/23/2020 11:59 AM	2021
3332	GROMACS	Feature	New	Normal	gmx helixorient doesn't have a -tu option to change time unit		01/22/2020 11:57 AM	
3328	GROMACS	Feature	New	Normal	Testing framework for task assignment		01/22/2020 09:48 AM	2021-refactoring
3318	GROMACS	Feature	In Progress	Normal	Use wrappers for the GPU buffer copy/allocations	Artem Zhmurov	01/23/2020 12:01 PM	2021-refactoring
3313	GROMACS	Feature	Accepted	Normal	Introduce and use opaque types for the DeviceStream and DeviceContext	Artem Zhmurov	01/23/2020 12:00 PM	2021-refactoring
3311	GROMACS	Feature	In Progress	Normal	GPU infrastructure development		03/20/2020 09:54 AM	2021-refactoring
3307	GROMACS	Feature	New	Normal	General interface for communication between simulation ranks		01/22/2020 03:22 PM	2021-refactoring
3298	GROMACS	Feature	New	Normal	start early PP work for first dimension of halo exchange		03/01/2020 01:36 PM	
3295	GROMACS	Feature	New	Normal	Expand gmxapi.modify_input use cases.	Eric Irrgang	01/16/2020 05:13 PM	2021-refactoring
3288	GROMACS	Feature	New	Normal	Use build system infrastructure instead of custom scripts to manage API levels.		02/26/2020 04:16 PM	2021-infrastructure-stable
3285	GROMACS	Feature	Resolved	Normal	Run simulations from the same tpr file with different random seeds		02/27/2020 11:22 PM	future
3283	GROMACS	Feature	Resolved	Normal	Support for the string method with swarms of trajectories in GROMACS		03/01/2020 01:16 PM	2021
3277	GROMACS	Feature	New	Normal	Allow testing feature that is partly implemented		12/31/2019 12:44 PM	2021
3242	GROMACS	Feature	New	Normal	Please do not remove the -nsteps flag		03/01/2020 01:59 PM	
3179	GROMACS	Feature	New	Normal	Clarify access to parallel data outputs	Eric Irrgang	10/26/2019 12:23 PM	
3177	GROMACS	Feature	New	Normal	Spack package management support		11/06/2019 06:37 PM	
3172	GROMACS	Feature	New	Normal	QM/MM Interface with CP2K	Dmitry Morozov	01/17/2020 12:18 PM	future
3160	GROMACS	Feature	Fix uploaded	High	implement direct comm for different src/target memory spaces	Alan Gray	02/14/2020 11:28 AM	2021-infrastructure-stable
3152	GROMACS	Feature	New	Normal	Infrastructure and patterns for expressing public interfaces		01/09/2020 05:19 PM	2021-infrastructure-stable
3149	GROMACS	Feature	New	Normal	Python user interface for obtaining simulation artifacts as files.	Eric Irrgang	10/15/2019 06:21 PM	
3148	GROMACS	Feature	New	Normal	Roadmap for gmxapi filesystem interactions.	Eric Irrgang	10/15/2019 06:23 PM	2021-infrastructure-stable
3147	GROMACS	Feature	New	Normal	gmxapi workflow checkpointing	Eric Irrgang	10/15/2019 06:18 PM	2021-infrastructure-stable
3140	GROMACS	Feature	New	Normal	Allow explicit input definition for gmxapi.operation function wrapper	Eric Irrgang	12/10/2019 02:00 PM	2021-infrastructure-stable
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	
3134	GROMACS	Feature	Feedback wanted	Normal	gmxapi Python exception names may need improvement	Eric Irrgang	10/13/2019 01:50 PM	
3126	GROMACS	Feature	New	Normal	State propagator GPU data manager		10/09/2019 02:42 PM	

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
3117	GROMACS	Feature	New	Normal	Coulomb FEP PME on GPU	Magnus Lundborg	02/17/2020 03:58 PM	2021-infrastructure-stable
3115	GROMACS	Feature	New	Normal	Device stream manager		10/04/2019 09:00 AM	
3114	GROMACS	Feature	New	Normal	Improve GPU update-constraints module	Artem Zhmurov	02/10/2020 04:30 PM	2021
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
3045	GROMACS	Feature	New	Low	Option to remove v-sites in trjconv?		07/19/2019 04:42 PM	
3038	GROMACS	Feature	New	Normal	Improvements to MD plugin development environment	Eric Irrgang	12/10/2019 01:58 PM	2021-infrastructure-stable
3032	GROMACS	Feature	Feedback wanted	Normal	Clean up dev-manual structure		12/11/2019 11:27 AM	2021-infrastructure-stable
3030	GROMACS	Feature	New	Normal	RST style guidelines		07/09/2019 03:38 PM	
3021	GROMACS	Feature	Feedback wanted	Normal	Completion of docs for GPU developments		03/02/2020 03:58 PM	2020.2
3020	GROMACS	Feature	New	Low	modernize DeviceBuffer and GPU memory management		08/13/2019 06:01 PM	
2996	GROMACS	Feature	In Progress	Normal	gmxapi execution model	Eric Irrgang	12/10/2019 01:57 PM	2021-infrastructure-stable
2994	GROMACS	Feature	New	Normal	Data flow topology in gmxapi 2020		12/11/2019 11:33 AM	2021-infrastructure-stable
2993	GROMACS	Feature	New	Normal	Scalar and structured type expression and definitions for API	Eric Irrgang	10/17/2019 09:55 AM	
2984	GROMACS	Feature	New	Normal	More Extensive Selections Examples	Dallas Warren	06/18/2019 11:50 PM	
2977	GROMACS	Feature	New	Normal	print DD load balancing improvement		06/13/2019 10:56 AM	
2975	GROMACS	Feature	New	Normal	LJ PME calculations on GPUs		06/12/2019 01:17 PM	
2967	GROMACS	Feature	New	Normal	GPU reallocateDeviceBuffer improvements		01/23/2020 12:15 PM	2021-refactoring
2961	GROMACS	Feature	New	Normal	How should Python package find GROMACS resources under various circumstances?		12/09/2019 10:47 AM	
2956	GROMACS	Feature	New	Normal	SAXS resolution		05/17/2019 09:58 AM	
2944	GROMACS	Feature	New	Normal	Roadmap for thermostats / barostats in new propagation/integration scheme	Michael Shirts	12/27/2019 04:00 PM	2021
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	
2915	GROMACS	Feature	In Progress	High	GPU direct communications		02/14/2020 12:48 PM	
2910	GROMACS	Feature	New	Normal	Mixed scaling for 1-4 interactions		04/10/2019 10:13 PM	
2896	GROMACS	Feature	Feedback wanted	Normal	Python packaging		01/16/2020 07:11 PM	2021-refactoring
2891	GROMACS	Feature	In Progress	Normal	PME/PP GPU communications		02/14/2020 12:40 PM	
2890	GROMACS	Feature	In Progress	Normal	GPU Halo Exchange		02/14/2020 12:41 PM	2021

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2866	GROMACS	Feature	New	Normal	Alternative non-bonded potentials	David van der Spoel	03/05/2019 03:50 PM	future
2860	GROMACS	Feature	New	Normal	Option for outputting min/max coordinates in gmx traj		02/08/2019 12:35 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
2806	GROMACS	Feature	New	Normal	SIMD algorithms for ARM SVE // nobonded cluster and others		12/27/2019 03:59 PM	2021
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
2774	GROMACS	Feature	New	Normal	Refactor shell code into its own integrator	David van der Spoel	12/27/2019 04:05 PM	2021
2761	GROMACS	Feature	New	Low	lincs-order 4 is too conservative for some force fields		11/16/2018 09:55 AM	
2755	GROMACS	Feature	New	Low	md5 sums and sha256, sha512 hashes	Benson Muite	02/19/2019 11:00 PM	
2739	GROMACS	Feature	New	Normal	Parallel continuous tempering and enhanced sampling feature		11/13/2018 11:36 PM	
2715	GROMACS	Feature	New	Normal	Avoid requesting the user to recompile gromacs for Intel OpenCL support		12/27/2019 04:06 PM	future
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		12/27/2019 04:41 PM	2021
2667	GROMACS	Feature	New	Normal	Suggested steps for calculating entropy in solution and binding	David van der Spoel	03/01/2020 01:35 PM	2020.2
2643	GROMACS	Feature	New	Low	mdp options and/or docs for anisotropic aspects of implementations		09/12/2018 02:23 PM	
2622	GROMACS	Feature	New	Low	Reduce severity of Berendsen warning		08/23/2018 11:16 PM	future
2601	GROMACS	Feature	New	Normal	Free energy calculations, soft-core potential	Vytautas Gapsys	02/10/2020 11:29 AM	future
2596	GROMACS	Feature	New	Normal	Constant potential method	Benson Muite	05/10/2019 09:54 AM	
2594	GROMACS	Feature	New	Normal	Multi-level GMX API	Prashanth Kanduri	02/22/2019 03:48 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	
2585	GROMACS	Feature	Resolved	Normal	Infrastructure supporting external API		12/11/2019 12:39 PM	
2581	GROMACS	Feature	Accepted	Normal	User interface for hybrid Monte Carlo		12/20/2019 12:24 PM	future
2579	GROMACS	Feature	New	Normal	Add dimensionality option to gmx trjconv -center		07/19/2018 04:53 PM	future
2574	GROMACS	Feature	New	Normal	iForceSchedule Abstraction	Prashanth Kanduri	03/29/2019 05:20 PM	future
2570	GROMACS	Feature	New	Normal	Better string formatting and printing		05/02/2019 12:20 PM	

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2556	GROMACS	Feature	New	Normal	make default selections suitable for DNA and RNA	Mark Abraham	06/20/2018 01:48 PM	
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
2545	GROMACS	Feature	New	Normal	Should grompp fix periodicity of input files?	David van der Spoel	10/03/2018 11:32 PM	future
2491	GROMACS	Feature	New	Low	Allow constant bias AWH simulations	Viveca Lindahl	06/05/2018 10:38 PM	future
2451	GROMACS	Feature	Resolved	Normal	Linear virtual sites with fixed distance	David van der Spoel	09/16/2019 01:15 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	
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
2354	GROMACS	Feature	New	Normal	develop configuration file support for control of task layout		09/19/2018 03:01 PM	future
2310	GROMACS	Feature	Accepted	Low	Let mdrun dump coordinates with non-finite energy		10/03/2018 09:47 PM	future
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
2254	GROMACS	Feature	Resolved	Normal	GPU extensions for Google Tests		10/06/2020 12:15 PM	
2248	GROMACS	Feature	New	Normal	Label all SIMD functions as pure/nodiscard		02/04/2019 04:49 AM	
2239	GROMACS	Feature	New	Normal	split libgromacs into base and full		01/07/2019 01:47 AM	
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	12/20/2019 12:11 PM	2021
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	
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	
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

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2139	GROMACS	Feature	New	Normal	More precise/explicit documentation conventions		01/07/2018 11:54 PM	
2137	GROMACS	Feature	New	Normal	Preliminary refactoring of constraints and update machinery.	Michael Shirts	03/11/2017 08:32 AM	future
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	
2111	GROMACS	Feature	In Progress	Normal	Implement Gaussian screening of electrostatics		02/23/2019 12:33 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
2090	GROMACS	Feature	New	Normal	redirecting stdout or stderr for testing	Mark Abraham	12/15/2016 03:15 AM	

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