

## Issues

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
3448	GROMACS	Bug	New	Normal	GMX 2020.1 - Multidir simulations can stop at different times when killed by job manager		03/23/2020 02:50 PM	
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	
3444	GROMACS	Bug	Resolved	Normal	do_dssp does not work(gmx 2020 and 2020.1)	Christian Blau	06/10/2020 02:45 PM	2020.2
3443	GROMACS	Bug	New	Normal	Bonded GPU kernel performance regression with 2020		03/15/2020 08:15 PM	
3442	GROMACS	Bug	Accepted	Normal	continuing mdrun with -deffnm and pulling does not work		03/15/2020 08:33 AM	
3441	GROMACS	Bug	Resolved	Normal	Ewald surface-epsilon is incorrect	Berk Hess	03/18/2020 11:15 PM	2020.2
3440	GROMACS	Bug	New	Normal	Multi-nodes run exits with error with openmpi/4.0.0		03/23/2020 02:10 PM	
3439	GROMACS	Feature	New	Normal	Optimize successive simulation segments		03/11/2020 01:42 PM	
3437	GROMACS	Task	New	Normal	Use builders to prepare modules	Pascal Merz	03/11/2020 07:05 AM	2021-infrastructure-stable
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
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
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

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3417	GROMACS	Feature	New	Normal	Make modular simulator feature-complete	Pascal Merz	03/23/2020 03:57 AM	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
3413	GROMACS	Bug	Feedback wanted	Normal	COMM Removal Failure in GROMACS 2020.1		03/12/2020 02:31 PM	
3412	GROMACS	Bug	New	Normal	Domain decomposition problems with Gromacs >2018		03/06/2020 04:10 PM	
3411	GROMACS	Bug	New	Normal	Nightly master release build failure		03/06/2020 11:44 AM	2021-infrastructure-stable
3410	GROMACS	Feature	New	Normal	Random Acceleration Molecular Dynamics (RAMD)	Bernd Doser	03/05/2020 03:22 PM	2021
3408	GROMACS	Bug	Fix uploaded	Normal	Gmxapi* tests segfault in rpmbuild	Eric Irrgang	03/23/2020 01:27 PM	2020.2
3405	GROMACS	Bug	Accepted	Normal	intermittent OpenCL regressiontest failures		03/02/2020 11:01 AM	
3403	GROMACS	Bug	Resolved	Normal	solvation free energy with couple-intramol set to no		12/10/2020 02:45 PM	
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
3398	GROMACS	Bug	New	Normal	Intermittent failure of non-bonded kernels when run using nvprof		02/25/2020 12:14 PM	
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
3392	GROMACS	Task	New	Low	Unify box correction for modular simulator	Pascal Merz	03/11/2020 05:20 PM	2021-infrastructure-stable
3387	GROMACS	Bug	New	Normal	Death test bug		02/20/2020 05:39 PM	
3385	GROMACS	Bug	New	Normal	FindLibStdCpp.cmake - wrong sanity check for clang		03/04/2020 06:59 PM	
3382	GROMACS	Task	Accepted	Normal	Split up t_inputrec		02/17/2020 05:28 PM	
3380	GROMACS	Bug	Resolved	Low	IBM VSX checks fail with gcc-10	Erik Lindahl	04/30/2020 01:30 PM	2020.2
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
3370	GROMACS	Task	New	High	Further improvements to GPU Buffer Ops and Comms		03/04/2020 01:38 PM	
3369	GROMACS	Feature	New	Normal	Add quote about "the truth"		02/05/2020 05:08 PM	
3368	GROMACS	Bug	New	Normal	Erroneous interplay between gmx rms command and atommass.dat: Can not find mass in database for atom MG in residue	Vedat Durmaz	02/05/2020 04:51 PM	future
3366	GROMACS	Task	New	Normal	Enforce compability of MdModules		02/28/2020 11:20 AM	

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3365	GROMACS	Task	New	Low	consider making GPU bonded work independent from nonbonded		03/01/2020 01:11 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	
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
3355	GROMACS	Feature	Accepted	Normal	New PME parallel (GPU) scheme	Jonathan Vincent	02/12/2020 11:58 AM	
3353	GROMACS	Task	New	Normal	Document gmx densmap output		01/23/2020 12:52 PM	
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
3350	GROMACS	Feature	New	Normal	GPU update-constraints performance	Artem Zhmurov	01/23/2020 11:59 AM	2021
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
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

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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
3334	GROMACS	Bug	New	Normal	Check for DD when increasing rlist is broken	Berk Hess	02/25/2020 03:28 PM	2020.2
3333	GROMACS	Bug	New	Normal	Assertion failure when trying to get unit test help	Paul Bauer	02/25/2020 10:16 AM	2021-infrastructure-stable
3332	GROMACS	Feature	New	Normal	gmx helixorient doesn't have a -tu option to change time unit		01/22/2020 11:57 AM	
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
3328	GROMACS	Feature	New	Normal	Testing framework for task assignment		01/22/2020 09:48 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
3318	GROMACS	Feature	In Progress	Normal	Use wrappers for the GPU buffer copy/allocations	Artem Zhmurov	01/23/2020 12:01 PM	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
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
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
3311	GROMACS	Feature	In Progress	Normal	GPU infrastructure development		03/20/2020 09:54 AM	2021-refactoring

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3310	GROMACS	Bug	Blocked, need info	Low	Thread affinity on Mac OS		02/27/2020 11:10 PM	
3309	GROMACS	Bug	New	Normal	-reprod: checkpoint reading bug and general considerations		02/27/2020 10:45 PM	
3308	GROMACS	Task	New	Normal	GPU update-constraints: Cycle counting for GPU launches		01/23/2020 11:54 AM	2021-infrastructure-stable
3307	GROMACS	Feature	New	Normal	General interface for communication between simulation ranks		01/22/2020 03:22 PM	2021-refactoring
3306	GROMACS	Task	New	Normal	Document gmx dos tool more clearly	Christian Blau	01/20/2020 02:31 PM	future
3305	GROMACS	Bug	New	Normal	Case gives FPE with Debug build when GPU update is enabled		01/21/2020 05:44 PM	
3304	GROMACS	Bug	New	Normal	Failure in Log Output for Expanded Ensemble Weights using Simulated Tempering in GROMACS 2019.5	Michael Shirts	03/01/2020 03:23 PM	2020.2
3301	GROMACS	Bug	New	Normal	pdb2gmx adding hydrogen		01/15/2020 10:17 PM	
3300	GROMACS	Task	New	Normal	Abandon docs/OpenCLTODOList.txt?		01/15/2020 02:46 PM	
3298	GROMACS	Feature	New	Normal	start early PP work for first dimension of halo exchange		03/01/2020 01:36 PM	
3297	GROMACS	Task	Resolved	Normal	Require gcc > 5		04/30/2020 11:00 AM	2021-infrastructure-stable
3295	GROMACS	Feature	New	Normal	Expand gmxapi.modify_input use cases.	Eric Irrgang	01/16/2020 05:13 PM	2021-refactoring
3294	GROMACS	Bug	New	Normal	multiple tests fail on fedora 31	Paul Bauer	02/28/2020 03:12 PM	2020.2
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	
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
3287	GROMACS	Task	New	Normal	Deprecate make_ndx, use select instead		01/23/2020 01:16 PM	
3285	GROMACS	Feature	Resolved	Normal	Run simulations from the same tpr file with different random seeds		02/27/2020 11:22 PM	future
3284	GROMACS	Bug	New	Normal	gmx msd cannot output two xvg files as suggested by command line option	Christian Blau	01/08/2020 04:50 PM	2021-infrastructure-stable
3283	GROMACS	Feature	Resolved	Normal	Support for the string method with swarms of trajectories in GROMACS		03/01/2020 01:16 PM	2021
3281	GROMACS	Bug	New	Normal	Test data directory GMX_RELEASE_ASSERT triggers		01/06/2020 08:07 PM	
3279	GROMACS	Task	New	Low	Provide more advice for building client software		03/02/2020 11:54 AM	
3277	GROMACS	Feature	New	Normal	Allow testing feature that is partly implemented		12/31/2019 12:44 PM	2021
3275	GROMACS	Task	New	Normal	Document Gitlab CI instead of Jenkins and releng	Paul Bauer	03/09/2020 05:55 PM	2021-infrastructure-stable
3274	GROMACS	Bug	New	Normal	Remove ARM NEON SIMD		12/28/2019 07:53 AM	2021-infrastructure-stable
3273	GROMACS	Bug	New	Normal	gmxapi setup.py complains too much		12/27/2019 06:42 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

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3266	GROMACS	Bug	New	High	gmx density show wrong symmetrize density profile using -symm?	Super duper	02/28/2020 08:24 AM	2020.2
3265	GROMACS	Bug	Blocked, need info	Low	regressiontests/complex fails on ppc64le	Erik Lindahl	01/09/2020 05:00 PM	
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	
3249	GROMACS	Bug	In Progress	Low	cmake bad tests for avx512 on AMD	Erik Lindahl	02/26/2020 05:00 PM	
3246	GROMACS	Bug	Accepted	Normal	GPU code misses settle error check, simulation crashes with segfault without any further output	Artem Zhmurov	12/20/2019 09:52 AM	2021-infrastructure-stable
3244	GROMACS	Bug	In Progress	Normal	center of mass motion removal with position restraints can lead to artifacts	Berk Hess	12/27/2019 10:40 AM	2021
3243	GROMACS	Bug	Feedback wanted	Normal	Convert GROMACS 1 OpenMP thread per rank fatal error into a warning		12/27/2019 10:31 AM	
3242	GROMACS	Feature	New	Normal	Please do not remove the -nsteps flag		03/01/2020 01:59 PM	
3240	GROMACS	Bug	New	Normal	segv with GPU DD direct communication with GPU update and -dlb off		01/15/2020 06:16 PM	
3239	GROMACS	Bug	New	Normal	GPU DD direct communication with GPU update error with RF		12/14/2019 05:15 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
3234	GROMACS	Bug	Accepted	Normal	Signal: Floating point exception Signal code: Floating point divide-by-zero	Erik Lindahl	12/16/2019 03:40 PM	
3233	GROMACS	Bug	New	Normal	clang-format incorrectly aligning altered function arguments		12/13/2019 12:41 PM	
3229	GROMACS	Task	New	Normal	Move checkpointing to the beginning of the MD step		01/16/2020 04:31 PM	2021-infrastructure-stable
3228	GROMACS	Bug	New	Normal	gmxapi.commandline_operation should gracefully handle input/output file arguments	Eric Irrgang	12/04/2019 03:27 PM	2021-infrastructure-stable
3227	GROMACS	Bug	New	Normal	solvate does not check return status of gmx_file_rename		12/04/2019 01:43 PM	
3224	GROMACS	Task	New	Normal	add regression test case large enough to miscalculated GPU grid launch cases		12/20/2019 01:18 PM	2021

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3223	GROMACS	Bug	New	Normal	unit test failures give verify -1		12/02/2019 11:58 AM	
3220	GROMACS	Task	New	Normal	change rolling pruning scheduling with GPU update		02/25/2020 03:41 PM	2021-infrastructure-stable
3219	GROMACS	Bug	Resolved	Normal	MANPATH setting is fragile		11/02/2020 11:45 AM	
3216	GROMACS	Task	New	Normal	improve CPU force reductions	Szilárd Páll	12/04/2019 09:24 PM	
3214	GROMACS	Bug	New	Normal	Out-of-bounds, overflow and incorrect outputs in gmx spatial		11/25/2019 04:11 PM	
3213	GROMACS	Bug	New	Normal	Having a local residuetypes.dat for custom force field		11/21/2019 09:18 PM	
3212	GROMACS	Task	New	Normal	Update regression tests for new kernel flavours		11/21/2019 11:50 AM	
3210	GROMACS	Bug	New	High	rerun does not reproduce dVcoul/dl		12/27/2019 10:45 AM	
3209	GROMACS	Bug	New	Normal	Interactive molecular dynamics with VMD becomes stuttering after reconnecting		11/19/2019 11:36 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
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	
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	
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
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	
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	

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
3172	GROMACS	Feature	New	Normal	QM/MM Interface with CP2K	Dmitry Morozov	01/17/2020 12:18 PM	future
3171	GROMACS	Task	New	Normal	schedule CPU H2D force contribution in separate stream		12/20/2019 08:33 AM	2021-infrastructure-stable
3166	GROMACS	Bug	New	Normal	Compilation failing on Ubuntu 19.04 with Cuda 10.1		10/19/2019 09:13 PM	
3165	GROMACS	Bug	New	Normal	task assignment silent abort		10/18/2019 07:46 PM	
3162	GROMACS	Task	New	Normal	Add virtual site support to GPU version of update-constraints.	Artem Zhmurov	01/23/2020 11:52 AM	2021-infrastructure-stable
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
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
3152	GROMACS	Feature	New	Normal	Infrastructure and patterns for expressing public interfaces		01/09/2020 05:19 PM	2021-infrastructure-stable
3150	GROMACS	Bug	New	Normal	gmxapi data type annotations are confusing and inadequate	Eric Irrgang	10/22/2019 03:08 PM	2021-infrastructure-stable
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
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
3141	GROMACS	Bug	New	Normal	gmxapi File placeholders missing from beta release	Eric Irrgang	12/10/2019 02:02 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
3139	GROMACS	Task	New	Normal	gmxapi Futures should be subscribable	Eric Irrgang	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 Irrgang	12/11/2019 11:25 AM	2021-infrastructure-stable
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	
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



#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
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	Resolved	Normal	OpenCL on Volta and Turing broken		02/27/2020 11:01 AM	2020.2
3124	GROMACS	Bug	New	Normal	significant performance loss due to DLB auto-off when PP/PME load >1		01/28/2020 02:44 PM	2021
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
3117	GROMACS	Feature	New	Normal	Coulomb FEP PME on GPU	Magnus Lundborg	02/17/2020 03:58 PM	2021-infrastructure-stable
3116	GROMACS	Bug	New	Normal	regressiontests/freeenergy core dumps on ppc64le	Paul Bauer	10/04/2019 10:52 PM	
3115	GROMACS	Feature	New	Normal	Device stream manager		10/04/2019 09:00 AM	
3114	GROMACS	Feature	New	Normal	Improve GPU update-constraints module	Artem Zhmurov	02/10/2020 04:30 PM	2021
3113	GROMACS	Bug	New	Low	Use of read_tps_conf is deprecated	Paul Bauer	10/01/2019 11:36 AM	2021-infrastructure-stable
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
3101	GROMACS	Bug	Blocked, need info	Normal	detect compilation failed	Erik Lindahl	12/27/2019 10:52 AM	
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
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		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
3075	GROMACS	Bug	New	Normal	Frozen atoms are moving	Erik Lindahl	12/27/2019 10:51 AM	
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

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
3071	GROMACS	Bug	Accepted	Normal	complex.nbnxn-ljpme-LB-geometric failing with OpenCL timing debug mode assertions	Szilárd Páll	02/25/2020 03:39 PM	2020.2
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		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
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	12/27/2019 04:22 PM	2021
3055	GROMACS	Bug	Feedback wanted	Normal	Error in gmx xpm2ps		08/22/2019 03:27 PM	
3054	GROMACS	Bug	New	Normal	Missing dihedral define		08/02/2019 05:47 PM	
3050	GROMACS	Bug	New	Low	Fix tests on Solaris	Vedran Miletic	02/27/2020 11:05 AM	2020.2
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	Feedback wanted	Normal	Set required versions for GROMACS 2021		02/20/2020 11:42 AM	
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	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	
3038	GROMACS	Feature	New	Normal	Improvements to MD plugin development environment	Eric Irrgang	12/10/2019 01:58 PM	2021-infrastructure-stable
3035	GROMACS	Task	New	Normal	Provide central logger in wrapper binary	Paul Bauer	09/06/2019 02:34 PM	2021-infrastructure-stable
3033	GROMACS	Task	In Progress	Normal	Clean up and modernize googletest bundling and usage		01/16/2020 04:50 PM	2021-refactoring
3032	GROMACS	Feature	Feedback wanted	Normal	Clean up dev-manual structure		12/11/2019 11:27 AM	2021-infrastructure-stable
3031	GROMACS	Task	New	Normal	evaluate the impact of particle order on PME		12/27/2019 04:29 PM	2021
3030	GROMACS	Feature	New	Normal	RST style guidelines		07/09/2019 03:38 PM	
3028	GROMACS	Bug	Feedback wanted	Normal	install fail on Centos 6		07/15/2019 12:32 PM	
3021	GROMACS	Feature	Feedback wanted	Normal	Completion of docs for GPU developments		03/02/2020 03:58 PM	2020.2

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
3020	GROMACS	Feature	New	Low	modernize DeviceBuffer and GPU memory management		08/13/2019 06:01 PM	
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	In Progress	Normal	gmxapi 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 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		12/27/2019 04:30 PM	2021
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	Resolved	Normal	Update Python detection		04/23/2020 04:45 PM	2021-infrastructure-stable
2997	GROMACS	Task	New	Normal	improve performance of alchemical free energy calculations		12/27/2019 04:31 PM	2021
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	
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
2987	GROMACS	Bug	New	Normal	assess the bonded GPU task assignment default		12/20/2019 01:06 PM	2021
2984	GROMACS	Feature	New	Normal	More Extensive Selections Examples	Dallas Warren	06/18/2019 11:50 PM	
2983	GROMACS	Task	New	Normal	better suited data-types for bonded GPU kernels		07/11/2019 04:32 PM	
2981	GROMACS	Bug	New	Normal	segfault in opencl build		06/18/2019 03:30 AM	
2980	GROMACS	Bug	New	Normal	taskassignment fails with unit tests when GPUs and custom number of ranks is used		06/17/2019 05:28 PM	
2978	GROMACS	Bug	New	Normal	Some suggestions about the gmx current tool		06/13/2019 12:41 PM	
2977	GROMACS	Feature	New	Normal	print DD load balancing improvement		06/13/2019 10:56 AM	
2976	GROMACS	Task	New	Normal	Basic math for Multidimensional arrays		12/27/2019 04:37 PM	2021
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 with OpenCL		02/25/2020 03:52 PM	2020.2
2967	GROMACS	Feature	New	Normal	GPU reallocateDeviceBuffer improvements		01/23/2020 12:15 PM	2021-refactoring

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
2965	GROMACS	Task	In Progress	Normal	Performance of GPU direct communications		02/14/2020 12:38 PM	2021
2961	GROMACS	Feature	New	Normal	How should Python package find GROMACS resources under various circumstances?		12/09/2019 10:47 AM	
2958	GROMACS	Bug	New	Normal	Compiling master (to become 2020) using CUDA 9.0		03/02/2020 03:57 PM	2020.2
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
2944	GROMACS	Feature	New	Normal	Roadmap for thermostats / barostats in new propagation/integration scheme	Michael Shirts	12/27/2019 04:00 PM	2021
2937	TNG trajectory library	Bug	New	Normal	tng_num_frames_get reports incorrect num frames		04/29/2019 11:30 AM	
2936	GROMACS	Task	New	Normal	introduce check that CPU-GPU transfers/assignments are made between compatible types		02/05/2020 03:57 PM	2021
2935	Support Platforms	Bug	New	High	redmine issue updates about gerrit uploads stopped working		06/11/2019 01:42 PM	current
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	
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
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	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	
2909	GROMACS	Task	New	Normal	consider implementing mechanisms to ensure pair lists are not used past their max lifetime		04/03/2019 05:14 PM	
2908	GROMACS	Task	New	Normal	Renaming things in nbxnm	Berk Hess	03/28/2019 10:10 AM	
2907	GROMACS	Bug	New	Normal	Gromacs autocompletion appears to be broken with ZSH		07/16/2019 04:46 AM	
2905	GROMACS	Task	New	Normal	Add a Jenkins configuration with std library assert		08/24/2019 05:22 PM	
2902	GROMACS	Bug	New	Normal	2019.1 equilibration issue? (Intel 2018u3)		04/30/2019 08:17 AM	
2898	GROMACS	Task	New	Low	Naming common variables		03/26/2019 11:46 PM	

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
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	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
2889	GROMACS	Task	New	Normal	update grompp warnings for brevity, usefulness and actionability	Mark Abraham	12/27/2019 04:38 PM	future
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 gm::Options more	Mark Abraham	12/20/2019 01:22 PM	2021
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	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	
2873	GROMACS	Bug	New	Normal	Simple way to get last frame from trajectory		02/28/2019 11:14 PM	
2872	GROMACS	Bug	New	Normal	gmx solvate and genion topology update		02/27/2019 10:18 AM	
2870	GROMACS	Bug	New	Normal	GPU detection error message missing from the output		03/05/2019 03:55 PM	
2869	GROMACS	Bug	New	Normal	GPU detection error only issued as a note to the log		03/05/2019 04:09 PM	
2866	GROMACS	Feature	New	Normal	Alternative non-bonded potentials	David van der Spoel	03/05/2019 03:50 PM	future
2864	GROMACS	Task	New	Normal	Building incompatibilities	Benson Muite	02/19/2019 02:00 PM	
2863	GROMACS	Task	New	Normal	improve PBC handling		03/11/2019 04:28 PM	
2860	GROMACS	Feature	New	Normal	Option for outputting min/max coordinates in gm traj		02/08/2019 12:35 AM	
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	
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	
2851	Support Platforms	Task	New	Normal	uninstall redmine checklist plugin		01/30/2019 03:33 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	gm make_ndx ignores last residue in case only CA's are present in GRO file		01/30/2019 06:16 AM	

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
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		01/16/2020 05:11 PM	2021
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
2832	GROMACS	Bug	New	Low	PaddedVector move operations broken	Mark Abraham	12/28/2019 10:40 AM	2021
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	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	
2806	GROMACS	Feature	New	Normal	SIMD algorithms for ARM SVE // nobonded cluster and others		12/27/2019 03:59 PM	2021
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	
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	12/27/2019 04:05 PM	2021
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	
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

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
2756	GROMACS	Task	In Progress	Normal	gmxapi integration testing		01/16/2020 05:12 PM	2021-refactoring
2755	GROMACS	Feature	New	Low	md5 sums and sha256, sha512 hashes	Benson Muite	02/19/2019 11:00 PM	
2754	GROMACS	Bug	New	Normal	Simulated Tempering seems to be broken	Michael Shirts	02/05/2019 03:58 PM	
2740	GROMACS	Bug	New	Normal	mdrun reports incorrect error with -bonded gpu without gpu	Mark Abraham	11/07/2018 01:59 PM	
2739	GROMACS	Feature	New	Normal	Parallel continuous tempering and enhanced sampling feature		11/13/2018 11:36 PM	
2735	GROMACS	Task	New	Normal	Allow gmx_genrestr to write correct position restraints for molecules after the first molecule	Joe Jordan	12/11/2019 09:26 AM	future
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	01/17/2020 08:40 AM	
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
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
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		12/02/2019 01:45 PM	2021-infrastructure-stable
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		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
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		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
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	03/01/2020 01:35 PM	2020.2

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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
2657	GROMACS	Bug	New	Normal	Biphasic tutorial		09/28/2018 10:02 AM	
2650	GROMACS	Task	New	Normal	revise OpenCL stack recommendations		12/31/2018 11:19 AM	future
2649	GROMACS	Bug	New	Normal	Virial calculation necessary for correct energy calculation on GPU		12/17/2018 02:32 PM	future
2645	GROMACS	Bug	New	Normal	Security		09/28/2018 01:16 PM	
2644	GROMACS	Task	New	Normal	Replace compute_globals	Mark Abraham	09/24/2018 05:51 PM	future
2643	GROMACS	Feature	New	Low	mdp options and/or docs for anisotropic aspects of implementations		09/12/2018 02:23 PM	
2637	GROMACS	Bug	New	High	gmx solvate tears apart molecules		09/11/2018 07:43 PM	
2632	GROMACS	Task	New	Low	make sure cmake defines proper hwloc versionc with cross-compilation enabled		12/03/2018 01:35 PM	future
2628	GROMACS	Bug	Resolved	Normal	GMXRC removes trailing colon from existing MANPATH		11/02/2020 11:45 AM	
2624	GROMACS	Bug	New	Normal	GPU build system not robust enough		09/05/2018 02:00 AM	
2622	GROMACS	Feature	New	Low	Reduce severity of Berendsen warning		08/23/2018 11:16 PM	future
2621	GROMACS	Task	New	Normal	Fine-Grained API to Describe Force Calculation and Neighbourhood Search	Prashanth Kanduri	08/22/2018 11:36 AM	future
2616	GROMACS	Task	New	Normal	Model for MD state		09/14/2018 05:12 PM	
2611	GROMACS	Bug	New	Normal	issues with gpu_utils-test with GMX_BUILD_UNITTESTS=OFF and on OSX		08/14/2018 07:03 PM	
2608	GROMACS	Task	New	Normal	Remove code duplication between OpenCL and CUDA		09/24/2018 12:47 PM	
2607	GROMACS	Bug	New	Normal	Grompp becomes extremely slow when many pull groups are present		08/11/2018 08:54 AM	
2606	GROMACS	Bug	New	Normal	Free Energy Calculation -- Function type Fourier Dih. Not implemented in ip_pert		08/10/2018 01:48 AM	
2603	GROMACS	Task	New	Normal	Add ability to properly check coordinate files during testing	Paul Bauer	10/15/2018 01:16 PM	future
2602	GROMACS	Bug	New	Low	build information gets outdated if build tree is reused		08/13/2018 09:04 PM	
2601	GROMACS	Feature	New	Normal	Free energy calculations, soft-core potential	Vytautas Gapsys	02/10/2020 11:29 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



#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
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	
2585	GROMACS	Feature	Resolved	Normal	Infrastructure supporting external API		12/11/2019 12:39 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	
2581	GROMACS	Feature	Accepted	Normal	User interface for hybrid Monte Carlo		12/20/2019 12:24 PM	future
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	
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	12/20/2019 12:21 PM	future

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
2535	GROMACS	Task	New	Normal	consider compiling opencl fft kernels once		05/31/2018 01:33 PM	
2532	GROMACS	Task	New	Normal	enable queue priorities in OpenCL		05/29/2018 02:29 PM	
2531	GROMACS	Task	New	Low	Consider optimizing tabulated data access on GPU		07/30/2018 12:31 PM	
2530	GROMACS	Task	New	Normal	consider using CUDA Driver API		09/23/2018 11:47 PM	future
2528	GROMACS	Task	New	Normal	PME GPU tuning		12/31/2018 11:18 AM	future
2527	GROMACS	Task	New	Normal	Rename GpuEventSynchronizer to something more fitting (after mergin PME OpenCL)		10/30/2018 04:06 AM	future
2526	GROMACS	Bug	New	Normal	Bug of gmx hbond		05/30/2018 03:12 PM	
2524	GROMACS	Task	New	Normal	struct alignment/packing for OpenCL host & device code		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
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		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
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		12/02/2019 01:22 PM	2021-infrastructure-stable
2480	GROMACS	Bug	New	Normal	pdb2gmx does not protonate correctly for united-atom Gromos	Mark Abraham	12/20/2019 12:17 PM	2021

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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
2473	GROMACS	Bug	New	Normal	mdrun sometimes stalls due to large coordinates with no constraints		04/04/2018 10:15 PM	
2469	GROMACS	Task	New	Normal	implement GPU timer reduction for reporting		03/27/2018 05:08 PM	
2468	GROMACS	Bug	New	Low	incorrect GPU timing reported with OpenCL and domain decomposition		12/17/2018 01:28 PM	future
2464	GROMACS	Task	New	Normal	GPU performance goals overview		03/26/2018 10:42 AM	
2463	GROMACS	Task	New	Low	PME GPU decomposition		03/26/2018 10:42 AM	
2462	GROMACS	Task	New	Normal	consider adding STL misuse tests		03/23/2018 01:23 AM	
2460	GROMACS	Bug	New	Normal	Allow inclusion of user libraries through CMake cache variables		03/28/2018 08:47 PM	
2456	GROMACS	Task	New	Normal	Add a pull module external potential tests		03/15/2018 03:02 PM	
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	
2451	GROMACS	Feature	Resolved	Normal	Linear virtual sites with fixed distance	David van der Spoel	09/16/2019 01:15 PM	

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