

Issues

| # | Project | Tracker | Status | Priority | Subject | Assignee | Updated | Target version |
|------|---------|---------|-------------|----------|--|---------------|---------------------|----------------------------|
| 3282 | GROMACS | Bug | Closed | High | Copyright message is not compatible with the clang-format | Mark Abraham | 01/09/2020 11:44 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 |
| 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 |
| 3207 | GROMACS | Task | Closed | Normal | Add cycle counting to StatePropagatorDataGpu | | 12/20/2019 08:17 AM | 2020-rc1 |
| 3236 | GROMACS | Task | New | Normal | GPU update-constraints: Pulling support | Artem Zhmurov | 01/23/2020 11:53 AM | 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 |
| 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 |
| 3314 | GROMACS | Task | Resolved | Normal | Platform agnostic DeviceStream | Artem Zhmurov | 03/20/2020 09:55 AM | 2021-refactoring |
| 3315 | GROMACS | Task | Resolved | Normal | Platform agnostic DeviceContext | Artem Zhmurov | 03/11/2020 04:15 PM | 2021-refactoring |
| 3316 | GROMACS | Task | Accepted | Normal | Context and Stream manager | 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 |
| 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 |
| 3320 | GROMACS | Task | In Progress | Normal | Remove duplicating D2H/H2D wrappers in NBNXM | 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 |
| 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 |
| 3323 | GROMACS | Task | In Progress | Normal | Rework the StatePropagatorDataGpu | Artem Zhmurov | 01/22/2020 09:50 AM | 2021-refactoring |
| 3324 | GROMACS | Task | New | Normal | Rework CMake handling of GPU code | | 01/22/2020 09:52 AM | 2021-refactoring |
| 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 |
| 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 |
| 3339 | GROMACS | Task | New | Normal | GPU LINCS: Warp-level synchronization for coupled constraints | Artem Zhmurov | 01/23/2020 11:55 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 |
| 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 |
| 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 |
| 3343 | GROMACS | Task | New | Normal | GPU SETTLE: Use different ordering for matrices. | 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 |
| 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 |
| 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 |

| # | Project | Tracker | Status | Priority | Subject | Assignee | Updated | Target version |
|------|---------|---------|-------------|----------|---|---------------|---------------------|----------------------------|
| 3347 | GROMACS | Task | Closed | Normal | GPU update-constraints: Reconsider naming | Artem Zhmurov | 01/23/2020 11:58 AM | 2021-refactoring |
| 3348 | GROMACS | Task | New | Normal | GPU LINCS and SETTLE: unify virial reduction | Artem Zhmurov | 01/23/2020 11:58 AM | 2021-infrastructure-stable |
| 3349 | GROMACS | Task | Closed | Normal | GPU update-constraints: Unify the PBC management. | Artem Zhmurov | 01/23/2020 11:59 AM | 2021-infrastructure-stable |
| 2885 | GROMACS | Feature | Closed | Normal | CUDA version of LINCS | Artem Zhmurov | 01/22/2020 11:49 AM | 2021-infrastructure-stable |
| 2886 | GROMACS | Feature | Closed | Normal | CUDA version of SETTLE | Artem Zhmurov | 01/22/2020 11:46 AM | 2021-infrastructure-stable |
| 2887 | GROMACS | Feature | Closed | Normal | CUDA version of Leap Frog algorithm | Artem Zhmurov | 12/02/2019 11:34 AM | 2020 |
| 2888 | GROMACS | Feature | Closed | Normal | CUDA Update and Constraints module | Artem Zhmurov | 01/22/2020 11:41 AM | 2021-infrastructure-stable |
| 3114 | GROMACS | Feature | New | Normal | Improve GPU update-constraints module | Artem Zhmurov | 02/10/2020 04:30 PM | 2021 |
| 3115 | GROMACS | Feature | New | Normal | Device stream manager | | 10/04/2019 09:00 AM | |
| 3126 | GROMACS | Feature | New | Normal | State propagator GPU data manager | | 10/09/2019 02:42 PM | |
| 3135 | GROMACS | Feature | New | Normal | Make GPU traits ino opaque types | | 10/14/2019 10:24 AM | |
| 3277 | GROMACS | Feature | New | Normal | Allow testing feature that is partly implemented | | 12/31/2019 12:44 PM | 2021 |
| 3311 | GROMACS | Feature | In Progress | Normal | GPU infrastructure development | | 03/20/2020 09:54 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 |
| 3318 | GROMACS | Feature | In Progress | Normal | Use wrappers for the GPU buffer copy/allocations | Artem Zhmurov | 01/23/2020 12:01 PM | 2021-refactoring |
| 3350 | GROMACS | Feature | New | Normal | GPU update-constraints performance | 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 |
| 3352 | GROMACS | Feature | New | Normal | GPU update-constraints feature support | Artem Zhmurov | 01/23/2020 11:59 AM | 2021 |
| 3372 | GROMACS | Bug | Closed | Normal | Re-enable RVec and float3 compatibility tests | Artem Zhmurov | 03/20/2020 09:54 AM | 2021-refactoring |
| 2898 | GROMACS | Task | New | Low | Naming common variables | | 03/26/2019 11:46 PM | |
| 3020 | GROMACS | Feature | New | Low | modernize DeviceBuffer and GPU memory management | | 08/13/2019 06:01 PM | |