

## Issues

| #    | Project | Tracker | Status   | Priority | Subject  | Assignee      | Updated             | Target version             |
|------|---------|---------|----------|----------|--|---------------|---------------------|----------------------------|
| 3324 | GROMACS | Task    | New      | Normal   | Rework CMake handling of GPU code  |               | 01/22/2020 09:52 AM | 2021-refactoring           |
| 3277 | GROMACS | Feature | New      | Normal   | Allow testing feature that is partly implemented   |               | 12/31/2019 12:44 PM | 2021                       |
| 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 |                            |
| 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 |                            |
| 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 |
| 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 |
| 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 |
| 3348 | GROMACS | Task    | New      | Normal   | GPU LINCS and SETTLE: unify virial reduction   | Artem Zhmurov | 01/23/2020 11:58 AM | 2021-infrastructure-stable |
| 3114 | GROMACS | Feature | New      | Normal   | Improve GPU update-constraints module  | Artem Zhmurov | 02/10/2020 04:30 PM | 2021                       |
| 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                       |
| 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           |
| 3316 | GROMACS | Task    | Accepted | Normal   | Context and Stream manager   | Artem Zhmurov | 01/22/2020 09:49 AM | 2021-refactoring           |

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| 3317 | GROMACS | Task    | Accepted    | Normal   | Improve testing of the GPU code  | Artem Zhmurov | 01/22/2020 09:49 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           |
| 3311 | GROMACS | Feature | In Progress | Normal   | GPU infrastructure development   |               | 03/20/2020 09:54 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           |
| 3318 | GROMACS | Feature | In Progress | Normal   | Use wrappers for the GPU buffer copy/allocations                                 | Artem Zhmurov | 01/23/2020 12:01 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           |
| 3323 | GROMACS | Task    | In Progress | Normal   | Rework the StatePropagatorDataGpu  | Artem Zhmurov | 01/22/2020 09:50 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           |
| 3207 | GROMACS | Task    | Closed      | Normal   | Add cycle counting to StatePropagatorDataGpu                                     |               | 12/20/2019 08:17 AM | 2020-rc1                   |
| 2887 | GROMACS | Feature | Closed      | Normal   | CUDA version of Leap Frog algorithm  | Artem Zhmurov | 12/02/2019 11:34 AM | 2020                       |
| 3347 | GROMACS | Task    | Closed      | Normal   | GPU update-constraints: Reconsider naming  | Artem Zhmurov | 01/23/2020 11:58 AM | 2021-refactoring           |
| 3372 | GROMACS | Bug     | Closed      | Normal   | Re-enable RVec and float3 compatibility tests                                    | Artem Zhmurov | 03/20/2020 09:54 AM | 2021-refactoring           |
| 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 |
| 2888 | GROMACS | Feature | Closed      | Normal   | CUDA Update and Constraints module   | Artem Zhmurov | 01/22/2020 11:41 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 |
| 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 |