<p>| #    | 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 | Jonathan Vincent      | 03/23/2020 02:50 PM          | 2020.1          |
| 3446 | GROMACS     | Task    | New        | Normal   | apply maintainability updates across all GPU kernels                     | Jonathan Vincent      | 03/19/2020 03:31 PM          | 2020.1          |
| 3445 | GROMACS     | Task    | New        | Normal   | create heuristic for c_skipNeutralAtoms                                   | Jonathan Vincent      | 03/17/2020 12:12 PM          |                |
| 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 -defnm 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    | New        | Normal   | Implement modular checkpointing for modular simulator                     | Pascal Merz           | 03/10/2020 10:39 PM          | 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 |</p>
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<td>Add reallocate(...) function that does not care about the contents of the buffer</td>
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<td>Use DeviceBuffer instead of native GPU types in NBNXM</td>
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<td>Data type for coordinates, xyzq data, LJ parameters data to use for GPU buffers</td>
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<td>Michael Shirts</td>
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<td>Expand gmxapi.modify_input use cases.</td>
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<td>GPU code misses settle error check, simulation crashes with segfault without any further output</td>
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<td>gmxapi.commandline_operation should gracefully handle input/output file arguments</td>
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<td>Tools should check that input is valid when first using it</td>
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<td>Remove extra D2H and H2D copies of coordinates when the COM motion is compensated.</td>
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<td>gmxapi.mdrun needs improved (and public) interface for attaching an MD extension.</td>
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