

## GROMACS - Task #2495

Task # 1781 (Accepted): re-design benchmarking functionality

### replace -noconfout with mdp option

04/27/2018 06:21 PM - Mark Abraham

|   |               |               |
|---|---------------|---------------|
| <b>Status:</b>  | Accepted      |               |
| <b>Priority:</b>  | Normal        |               |
| <b>Assignee:</b>  | Mark Abraham  |               |
| <b>Category:</b>  | mdrun         |               |
| <b>Target version:</b>  | 2021          |               |
| <b>Difficulty:</b>  | uncategorized |               |
| <b>Description</b>  |               |               |
| At <a href="https://gerrit.gromacs.org/#/c/7451">https://gerrit.gromacs.org/#/c/7451</a> Berk suggested, and Erik and I agreed, that we replace mdrun -noconfout with an mdp option, which is on by default so that normal behaviour that normal users see stays the same. This option can be turned off when it is useful, e.g. in an .mdp file for benchmark tpr. |               |               |
| <b>Related issues:</b>  |               |               |
| Related to GROMACS - Task #2569: announce deprecations in GROMACS 2019  |               | <b>Closed</b> |
| Related to GROMACS - Task #2169: remove 'continuation' mdp option   |               | <b>New</b>    |

### Associated revisions

#### Revision cf2d8336 - 10/13/2018 09:53 PM - Mark Abraham

Deprecate various functionality in GROMACS 2019

Published a deprecation policy.

Updated the release notes to refer also to previously deprecated features.

Announced intent to change some functionality:

- gmX mdrun -membed options (but not feature)
- gmX mdrun -rerun option (but not feature)
- integrator .mdp field will contain only integrators
- gmX do\_dssp to be replaced by gmX dssp
- gmX trjconv and friends to be split and rewritten

List of newly deprecated functionality:

- conversion of aromatic rings to virtual sites
- gmX mdrun -table options (but not feature)
- gmX mdrun -gcom option and feature
- gmX mdrun -nsteps option and feature
- gmX mdrun -nsteps -resetstep -resetthway moved to a gmX benchmark tool
- gmX mdrun -confout removed

Also updated release notes for functionality removed in GROMACS 2019.

Refs #2495, #1781

Fixes #2569, #1925

Change-Id: I1d00859d0f15409a472984f5a65347a50c71ad17

### History

#### #1 - 09/19/2018 03:14 PM - Mark Abraham

- Related to Task #2569: announce deprecations in GROMACS 2019 added

#### #2 - 09/19/2018 03:15 PM - Mark Abraham

The proposal to have gmX benchmark replace gmX mdrun for that use case is a natural way to have the default for -c to be on or off in the two relevant cases.

**#3 - 09/19/2018 04:19 PM - Szilárd Páll**

BTW, there seems to be no documentation on what is the *intended* use of the confout file -- and perhaps have a conversation whether those functions can be served better by other mechanism in the future (e.g. checking that a simulation has completed).

**#4 - 09/20/2018 09:12 AM - Berk Hess**

Having the benchmark tool removes the (short term) need for an mdp option for confout.gro.

But the confout.gro file is an awkward construct for all its current uses. For capturing the state of the system for transfer between EM and MD tng would be a better option. For transfer between MD and MD a checkpoint works, although I'm not sure what happens when you change coupling algorithms etc.

And indeed we need a proper way of signaling that a simulation has finished successfully.

**#5 - 10/05/2018 11:49 AM - Gerrit Code Review Bot**

Gerrit received a related patchset '1' for Issue [#2495](#).

Uploader: Mark Abraham ([mark.j.abraham@gmail.com](mailto:mark.j.abraham@gmail.com))

Change-Id: gromacs~master~11d00859d0f15409a472984f5a65347a50c71ad17

Gerrit URL: <https://gerrit.gromacs.org/8488>

**#6 - 10/12/2018 10:34 PM - Mark Abraham**

- *Target version changed from 2019 to 2020*

**#7 - 10/12/2018 10:36 PM - Mark Abraham**

- *Related to Task #2169: remove 'continuation' mdp option added*

**#8 - 12/20/2019 12:18 PM - Paul Bauer**

- *Status changed from New to Resolved*

**#9 - 12/28/2019 10:39 AM - Paul Bauer**

- *Status changed from Resolved to Accepted*

- *Target version changed from 2020 to 2021*

I think this should instead be kept open for 2021