

## GROMACS - Task #2059

### Separate different types of data in t\_state

10/15/2016 12:44 PM - Berk Hess

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|--|---------------|
| <b>Status:</b>   | In Progress   |
| <b>Priority:</b>   | Normal        |
| <b>Assignee:</b>   |               |
| <b>Category:</b>   | core library  |
| <b>Target version:</b>   | 2021          |
| <b>Difficulty:</b>   | uncategorized |
| <b>Description</b>   |               |
| <p>In mdrun there are 3 different types of state information:</p> <ol style="list-style-type: none"><li>1) The microstate of the simulated system</li><li>2) History information for output, e.g. energy statistics</li><li>3) The state of the mdrun machinery</li></ol> <p>Currently types 1) and 2) are both stored in t_state. A little of of type 3) is stored in the checkpoint file. Since types 1) and 2) serve very different purposes and are used mostly in different places in the code, they should be separated. My proposal is to only have data of type 1) in t_state. Some data, like energyhistory_t are clearly of type 2), but for other data, such as free-energy and swap data, this is not clear to me.</p> |               |

#### Associated revisions

##### Revision bd9f965f - 10/15/2016 12:48 PM - Berk Hess

Move energyhistory\_t out of t\_state

We have three different types of states in mdrun:

- 1) the microstate of the system we are simulating
- 2) history information for output
- 3) the state of the simulation machinery in mdrun

The struct energyhistory\_t clearly belongs to 2) and is therefore moved out of t\_state, which should eventually only contain 1).

TODO: Consider what to do with the other structs in t\_state that (also) store history rather than the state of the simulated system.

Note: reverts recent commit ec827264

Part of #2059.

Change-Id: Ie84a19efcd0a170c0aaafe18c06275b7fb15244a

##### Revision 036fc219 - 11/23/2016 03:17 PM - Berk Hess

Use templating in checkpoint.cpp

The low level int, real and double writing routines have been converted to a single template function. The listing functionality has been moved to a separate function. Added functions for processing more std::vector types.

Also fixes a bug causing memory corruption in gmx dump -cp.

Part of #2059.

Change-Id: Ia48e57841c7a2dfaa3aefd1f43f0cdc9c0034119

##### Revision f9399260 - 11/23/2016 03:18 PM - Berk Hess

Convert energyhistory\_t to use std::vector

This change converts energyhistory\_t and its child struct delta\_h\_history\_t to classes that use std::vector. Thus the init and done routines and energyhistory.cpp are removed.

Part of #2059.

Change-Id: leb1f43d18187d4f8de5a21d043bccdcf6686280d

#### Revision 1ecd43b0 - 05/22/2017 11:42 AM - Berk Hess

Introduce ObservablesHistory container

Introduces a ObservablesHistory class and moved energyhistory\_t, edsamstate\_t and swapstate\_t into this.

TODO: Move more observables history from t\_state into this container.

Also added documentation in state.h.

Part of #2059.

Change-Id: lc1efd95c5be2dede137763bfd24e3fb7d676eadd

## History

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### #1 - 10/15/2016 12:48 PM - Gerrit Code Review Bot

Gerrit received a related patchset '2' for Issue [#2059](#).

Uploader: Berk Hess ([hess@kth.se](mailto:hess@kth.se))

Change-Id: le84a19efcd0a170c0aaafe18c06275b7fb15244a

Gerrit URL: <https://gerrit.gromacs.org/6274>

### #2 - 10/15/2016 03:47 PM - Michael Shirts

Some data, like energyhistory\_t are clearly of type 2), but for other data, such as free-energy and swap data, this is not clear to me.

Great question. df\_history is required by the expanded ensemble subroutines to be able to decide how to update the weights for a number of weight-updating methods; for example, the Wang-Landau histogram. For checkpointing, then if this history is required to be able to restart. But I don't know that per se it needs to be stored as the state. It sort of made sense at the time (the state of the simulation, meaning all the information needed to determine what it would do next at an algorithmic level) would include the information in df\_history. If we think of the state as only the Markovian state of the simulation, then it wouldn't belong there.

Otherwise, df\_history it's only used for output.

One other thing -- it turns out it would be rather nice to be able to read the df\_history when restarting a simulation even when not using checkpoints. If running wang-landau, one might want to run a swarm of short trajectories (something we are working on now), and if the time for the histogram to flatten is too long, then you never really get the WL weights to converge.

Berk, we should set up a time to talk expanded ensemble methods at some point. Some interesting relationships between Lidmar's approach (which I know you've been using), MBAR, and provably optimally convergent methods are emerging (some but not all published). All of which might affect what would appear in df\_history and how it is used.

### #3 - 10/17/2016 10:59 AM - Michael Shirts

```
real *Tij;          / transition matrix /  
real **Tij_empirical; / Empirical transition matrix */
```

These definitely are descriptive, not required to define a non-markovian state for wang-landau, so could go somewhere else.

### #4 - 10/18/2016 10:29 AM - Gerrit Code Review Bot

Gerrit received a related patchset '4' for Issue [#2059](#).

Uploader: Berk Hess ([hess@kth.se](mailto:hess@kth.se))

Change-Id: la48e57841c7a2dfaa3aefd1f43f0cdc9c0034119

Gerrit URL: <https://gerrit.gromacs.org/6278>

### #5 - 10/18/2016 10:58 AM - Gerrit Code Review Bot

Gerrit received a related patchset '4' for Issue [#2059](#).

Uploader: Berk Hess ([hess@kth.se](mailto:hess@kth.se))

Change-Id: leb1f43d18187d4f8de5a21d043bccdcf6686280d

Gerrit URL: <https://gerrit.gromacs.org/6279>

### #6 - 10/18/2016 03:14 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue [#2059](#).

Uploader: Berk Hess ([hess@kth.se](mailto:hess@kth.se))

Change-Id: lc1efd95c5be2dede137763bfd24e3fb7d676eadd

Gerrit URL: <https://gerrit.gromacs.org/6280>

**#7 - 04/23/2017 08:13 PM - Mark Abraham**

- Target version changed from 2018 to 2019

I imagine there's more to do here, but not for this release.

**#8 - 05/10/2017 11:12 AM - Gerrit Code Review Bot**

Gerrit received a related DRAFT patchset '1' for Issue [#2059](#).

Uploader: Berk Hess ([hess@kth.se](mailto:hess@kth.se))

Change-Id: gromacs~master~ldeda2b0bf6bdd0eec1332549759bceb5ead87a5f

Gerrit URL: <https://gerrit.gromacs.org/6620>

**#9 - 05/10/2017 03:02 PM - Gerrit Code Review Bot**

Gerrit received a related patchset '13' for Issue [#2059](#).

Uploader: Berk Hess ([hess@kth.se](mailto:hess@kth.se))

Change-Id: gromacs~master~lc1efd95c5be2dede137763bfd24e3fb7d676eadd

Gerrit URL: <https://gerrit.gromacs.org/6280>

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

- Target version changed from 2019 to 2020

**#11 - 12/20/2019 12:09 PM - Paul Bauer**

@Berk can this be considered to be resolved for 2020?

**#12 - 12/27/2019 04:42 PM - Paul Bauer**

- Target version changed from 2020 to 2021

I guess not