

GROMACS - Bug #2767

grompp warns about md + FEP even for fully coupled states

11/19/2018 05:33 AM - Mark Abraham

Status: Closed	
Priority: Normal	
Assignee: Berk Hess	
Category: preprocessing (pdb2gmx,grompp)	
Target version: 2020-rc1	
Affected version - extra info: probably all versions since about 5.0	Difficulty: uncategorized
Affected version: 2018.4	
Description	
gmx grompp with FEP .mdp inputs and non-SD integrators issues	
<pre>WARNING 1 [file grompp.mdp, line 62]: For proper sampling of the (nearly) decoupled state, stochastic dynamics should be used</pre>	
It does so even for a fully coupled state. We should not be issuing warnings when there's no data to support that, because that will train users to use -maxwarn.	
We should check if this warning is still appropriate	
<ul style="list-style-type: none">• at least check the git history for which Redmine added it - is full VDW but no charge OK?• is the warning based on ancient implementations and needs updating?	
If we keep it, it should be sensitive to the calculation being done. For example, even slow growth (TI) starting from a not-nearly decoupled state should not issue it. FEP should only issue it for suitable values of lambda (if any).	

Associated revisions

Revision 253b576b - 12/18/2019 11:34 AM - Berk Hess

Change grompp decoupling SD warning to note

The warning that grompp issues when decoupling a molecule without the use of the SD integrator has been changed to a note, since there are valid use cases for using normal MD when not running in the completely decoupled state.

Note that checking for actual decoupled VdW states requires a lot of code and would still not be 100% correct.

Fixes #2767

Change-Id: I55c84afcbcb7b19bdb8a7a8bc586a65c50f8d0c1

History

#1 - 11/19/2018 05:34 AM - Mark Abraham

- File *fep-warning-repro.tgz* added

#2 - 11/19/2018 11:41 AM - Berk Hess

The user can manually modify the topology to decouple a molecule. Do we want to check for that? Or do we rather want to reduce false positives and accept some false negatives? Then we would only need to check if we have a fully decoupled state, i.e. `couple-lam0/1 = none` with `lambda=0/1`.

#3 - 12/06/2019 02:43 PM - Berk Hess

- Status changed from *New* to *Fix uploaded*

- Assignee set to *Berk Hess*

- Target version changed from *2020* to *2019.5*

Uploaded a "fix" that changes the warning to a note.

#4 - 12/18/2019 11:45 AM - Berk Hess

- Status changed from Fix uploaded to Resolved

Applied in changeset [253b576b2c6581490190f62912da72f4e3744f58](#).

#5 - 12/19/2019 10:13 AM - Berk Hess

- Target version changed from 2019.5 to 2020-rc1

#6 - 12/20/2019 08:17 AM - Paul Bauer

- Status changed from Resolved to Closed

Files

fep-warning-repro.tgz	5.88 MB	11/19/2018	Mark Abraham
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