GROMACS - Feature #976

Improve environment variable names

07/24/2012 04:03 AM - Justin Lemkul

<table>
<thead>
<tr>
<th>Status:</th>
<th>Closed</th>
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<tbody>
<tr>
<td>Priority:</td>
<td>Normal</td>
</tr>
<tr>
<td>Assignee:</td>
<td>Rossen Apostolov</td>
</tr>
<tr>
<td>Category:</td>
<td>documentation</td>
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<tr>
<td>Target version:</td>
<td>5.0</td>
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<td>Difficulty:</td>
<td>uncategorized</td>
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Description

While documenting various environment variables, I encountered several that have very generic names that could be improved by making them more descriptive. Many are involved in the QM interface, but there are others. Some of the env. vars. that could be made more explicit (in my opinion) are:

ACC  
BASENAME  
MEM  
NCPUS  
SASTEP  
STATE  
TOTAL  
VERBOSE  
WHERE  
LOGO  

Even prefixing them with GMX_ and some indication of how they're used (e.g. GMX_QM_ORCA_BASE instead of BASENAME, GMX_ENER_VERBOSE instead of VERBOSE, etc) would make them much better. I will suggest this for inclusion in 5.0/master to avoid largely cosmetic changes to the code.

Associated revisions

Revision da96f04b - 06/12/2014 06:27 PM - Rossen Apostolov

Cleanup environment variables.

Renamed variables to more descriptive names and removed unused ones.

Fixes #976.

Change-id: l0c17443c93efe581bf728f783893181e5a7f8ed8

History

#1 - 07/24/2012 04:03 AM - Justin Lemkul
- Assignee deleted (Justin Lemkul)

#2 - 05/13/2014 10:07 AM - Mark Abraham
- Target version changed from 5.0 to future

#3 - 06/12/2014 06:28 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue #976.
Uploader: Rossen Apostolov (rossen@kth.se)
Change-id: l0c17443c93efe581bf728f783893181e5a7f8ed8
Gerrit URL: https://gerrit.gromacs.org/3588

#4 - 06/12/2014 06:29 PM - Rossen Apostolov
- Status changed from New to Fix uploaded

This should be a rather extensive list of such variables.
#5 - 06/13/2014 02:15 PM - Rossen Apostolov
- Status changed from Fix uploaded to Resolved
- % Done changed from 0 to 100

Applied in changeset da96f04b93b8c407c66f641afb7b2f79d5b2f811.

#6 - 06/13/2014 02:35 PM - Erik Lindahl
- Status changed from Resolved to Closed

#7 - 07/15/2014 11:16 AM - Teemu Murtola
- Assignee set to Rossen Apostolov
- Target version changed from future to 5.0