GROMACS - Bug #1286
QM/MM Build Broken

06/19/2013 01:46 PM - 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>Justin Lemkul</td>
</tr>
<tr>
<td>Category:</td>
<td>build system</td>
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<tr>
<td>Target version:</td>
<td>4.6.3</td>
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<tr>
<td>Difficulty:</td>
<td>uncategorized</td>
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<tr>
<td>Affected version</td>
<td>4.6.2</td>
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Description
As reported on gmx-users, installing QM/MM support with ORCA silently fails. Installation proceeds without error, but the mdrun binary gives a fatal error (Ab-initio calculation only supported with Gamess, Gaussian or ORCA.) From config.h, I can see that GMX_QMMM_ORCA is never #defined, and it appears that the environment variable is never set. I have found that GMX_QMMM_ORCA is not listed in config.h.cmakein, which causes the problem. I will upload a patch to Gerrit to fix this issue, but it appears that the ORCA QM/MM interface still does not actually work, since the mdrun executable fails with a fatal error, but that's a separate issue.

Associated revisions
Revision 0e4e3ca8 - 06/28/2013 05:16 AM - Justin Lemkul
Fixes to config.h.cmakein to set GMX_QMMM_ORCA.
Installing using ORCA for QM calculations would proceed without any issue, but the mdrun executable was nonfunctional because GMX_QMMM_ORCA was never #defined, so the code was not correctly compiled.
Fixes #1286
Change-id: I230ded2d3cdbd9c5fc3e865d0b20049effb16766

History
#1 - 06/23/2013 10:38 PM - Justin Lemkul
- Status changed from New to Fix uploaded

#2 - 06/28/2013 05:20 AM - Justin Lemkul
- Status changed from Fix uploaded to Resolved
- % Done changed from 0 to 100

Applied in changeset 0e4e3ca811336600d31da2f29c19709a258fd92a.

#3 - 12/03/2013 04:17 PM - Rossen Apostolov
- Status changed from Resolved to Closed

05/03/2020