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: i230ded2d3cdcd9c5fc3e865d0b20049effb16766

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