### GROMACS - Bug #2800

gmx analyze cannot use lmfit

12/11/2018 04:10 PM - Magnus Lundborg

<table>
<thead>
<tr>
<th>Status:</th>
<th>Closed</th>
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<th>Normal</th>
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<tr>
<td>Assignee:</td>
<td></td>
<td>Category:</td>
<td>analysis tools</td>
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<td>Target version:</td>
<td>2019</td>
<td>Difficulty:</td>
<td>uncategorized</td>
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**Description**

When using the -fitfn option of gmx analyze I get:

Fatal error: This build of GROMACS was not configured with support for lmfit, so the requested fitting cannot be performed. See the install guide for instructions on how to build GROMACS with lmfit supported.

I've tried building GROMACS both with the default (internal) and with an external 7.0 version of lmfit, but it does not seem to make any difference.

**Associated revisions**

Revision 07ea0377 - 12/14/2018 02:23 PM - Magnus Lundborg

Set HAVE_LMFIT properly

The HAVE_LMFIT was only set in the local scope.

Fixes #2800

Change-Id: I34bd3dc1896526c09c6808c7020d3a492c4c8f31

**History**

#1 - 12/11/2018 05:18 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue #2800.
Uploader: Magnus Lundborg (magnus.lundborg@sciifelab.se)
Change-Id: gromacs~release-2019~I34bd3dc1896526c09c6808c7020d3a492c4c8f31
Gerrit URL: https://gerrit.gromacs.org/8810

#2 - 12/14/2018 11:39 AM - Paul Bauer

The fix seems fine to me, but can you upload a minimal test case as well?
So we may be able to add another unit test

#3 - 12/14/2018 12:48 PM - Paul Bauer

- Status changed from New to Fix uploaded

#4 - 12/14/2018 02:30 PM - Magnus Lundborg

- Status changed from Fix uploaded to Resolved

Applied in changeset 07ea0377472fc18c16fb3d3db38c7cb1f63c484.

#5 - 12/14/2018 02:41 PM - Paul Bauer

- Status changed from Resolved to Closed