GROMACS - Bug #795
mdrun segfaults for npme > np
08/24/2011 04:31 PM - Carsten Kutzner

<table>
<thead>
<tr>
<th>Status:</th>
<th>Closed</th>
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<tbody>
<tr>
<td>Priority:</td>
<td>Low</td>
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<tr>
<td>Assignee:</td>
<td>Carsten Kutzner</td>
</tr>
<tr>
<td>Category:</td>
<td>mdrun</td>
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<tr>
<td>Target version:</td>
<td>4.5.5</td>
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<td>Affected version - extra info:</td>
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<td>Affected version:</td>
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**Description**
Currently, Gromacs 4.5.4 gives a segfault if one runs mpirun -np 8 mdrun_mpi -npme 120 with no warning of the source of the problem. Obviously npme>nnodes is a bad setup, but a check would be nice.

The cause for this behavior is:
cr->npmenodes is set in mdrun.c right after the command line args are parsed, and in the code there is also a comment that npme>nnodes should not cause a problem at that point.

However, if npme>nnodes, in init_domain_decomposition / dd_choose_grid / optimize_ncells the number of pp nodes = nnodes-npme turns out to be negative such that in factorize the memory allocation does not work.

**Associated revisions**
Revision e230816f - 08/25/2011 11:12 AM - Carsten Kutzner
Instead of a segv, mdrun now gives an error msg if npme>np, fixes #795
Change-Id: l2e93bbcf45ace215d6237354559b8750628a13d6

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**History**
#1 - 08/24/2011 05:29 PM - Carsten Kutzner
- Status changed from New to 3
- % Done changed from 0 to 100

I have added appropriate checks in domdec_setup.c

#2 - 08/26/2011 10:47 AM - Carsten Kutzner
- Status changed from 3 to Closed