

## GROMACS - Bug #2303

Feature # 2054 (Accepted): PME on GPU

### PME GPU opt-in mixed mode is broken with PME tuning

11/25/2017 12:42 PM - Aleksei lupinov

<b>Status:</b> Closed	
<b>Priority:</b> High	
<b>Assignee:</b> Aleksei lupinov	
<b>Category:</b> core library	
<b>Target version:</b> 2018	
<b>Affected version - extra info:</b>	<b>Difficulty:</b> simple
<b>Affected version:</b> git master	
<b>Description</b> As Berk reports, infinite energies are produced after the tuning grid switch. In debug build GPU gather asserts on invalid grid values as well. Will look into this, and enhance the PME test to test the tuning mode as well (with small nstlist to trigger the grid switching, and disabled rec. energy checks).	

#### Associated revisions

##### Revision 3c1cf95c - 11/27/2017 06:39 PM - Aleksei lupinov

Add tests for PME tuning and fix mixed PME mode with tuning

Fixes #2303

Change-Id: Id9acd3d9b01b585d772b2009dcea9a9e0b8b0539

#### History

##### #1 - 11/25/2017 12:43 PM - Aleksei lupinov

- Parent task changed from #2124 to #2054

##### #2 - 11/27/2017 03:54 PM - Gerrit Code Review Bot

Gerrit received a related patchset '2' for Issue [#2303](#).

Uploader: Aleksei lupinov ([a.yupinov@gmail.com](mailto:a.yupinov@gmail.com))

Change-Id: gromacs~master~Id9acd3d9b01b585d772b2009dcea9a9e0b8b0539

Gerrit URL: <https://gerrit.gromacs.org/7236>

##### #3 - 11/27/2017 07:08 PM - Aleksei lupinov

- Status changed from In Progress to Resolved

Applied in changeset [3c1cf95c2207c1fb7413f5f46cc833597ea48d3d](#).

##### #4 - 11/28/2017 08:18 AM - Aleksei lupinov

- Status changed from Resolved to Closed