

## GROMACS - Task #2425

### testing multisim with multiple ranks per simulation

02/27/2018 04:42 PM - Mark Abraham

<b>Status:</b>	New	
<b>Priority:</b>	Normal	
<b>Assignee:</b>	Mark Abraham	
<b>Category:</b>	testing	
<b>Target version:</b>	2021	
<b>Difficulty:</b>	uncategorized	
<b>Description</b>		
As <a href="#">#2403</a> shows, we have a gap in testing coverage (and IIRC there were past issues when refactoring multisim and multiple ranks per simulation)		
<b>Related issues:</b>		
Related to GROMACS - Bug #2403: Multidir sim with #mpiranks = 2*#sim fails		<b>Closed</b>

#### History

##### #1 - 02/27/2018 04:43 PM - Mark Abraham

I have some work in progress, but no time available right now.

##### #2 - 02/27/2018 04:43 PM - Mark Abraham

- Related to Bug #2403: Multidir sim with #mpiranks = 2\*#sim fails added

##### #3 - 03/02/2018 12:42 PM - Szilárd Páll

Mark Abraham wrote:

As [#2403](#) shows, we have a gap in testing coverage (and IIRC there were past issues when refactoring multisim and multiple ranks per simulation)

The gap is actually somewhat, I'd suggest broadening this to covering better all domain/multi-rank decomposition modes (1/2/3 dim DD +/- separate PME with/without multisim).

##### #4 - 11/29/2018 11:20 AM - Mark Abraham

- Target version changed from 2019 to 2020

We need better infrastructure and design in order to be able to cover both one-rank per sim and multiple-ranks per sim, and definitely more work for the cases Szilard suggests (and anyway we will not be able to fully cover a whole multi-dimensional array of test cases).

##### #5 - 12/20/2019 12:13 PM - Paul Bauer

- Target version changed from 2020 to 2021