

GROMACS - Bug #3214

Out-of-bounds, overflow and incorrect outputs in gmx spatial

11/25/2019 04:11 PM - Shun Sakuraba

Status: New	
Priority: Normal	
Assignee:	
Category: analysis tools	
Target version:	
Affected version - extra info:	Difficulty: uncategorized
Affected version: 2019.4	
Description	
<p>While using gmx spatial I encountered multiple problems. After reading the source I also found multiple problems that corrupts the results of the analysis (especially the wrong number of grid counts and incorrect coordinates are problematic ones).</p> <ol style="list-style-type: none">1. Out-of-bound memory writes2. Confusing error message when the coordinate is exactly on the boundary (happens with .xtc files)3. Norm may become negative due to overflow4. Having negative iIGNOREOUTER (default -1) led to incorrect number of grid points5. The coordinates of the grid points were incorrect especially when iIGNOREOUTER is non-zero6. Norm calculation was incorrect <p>Attached patches should solve the problems.</p>	

Files

0001-Fixed-out-of-bound-access-in-gmx-spatial.patch	1.42 KB	11/25/2019	Shun Sakuraba
0003-Fixed-multiple-issues-with-gmx-spatial.patch	5.99 KB	11/25/2019	Shun Sakuraba
0002-Fixed-incorrect-boundary-conditions-in-gmx-spatial.patch	2.18 KB	11/25/2019	Shun Sakuraba