

## GROMACS - Bug #3066

### Gauss transform and density fit classes should operate on real values instead of float

08/26/2019 11:53 AM - Christian Blau

<b>Status:</b> New	
<b>Priority:</b> Normal	
<b>Assignee:</b> Christian Blau	
<b>Category:</b> core library	
<b>Target version:</b>	
<b>Affected version - extra info:</b>	<b>Difficulty:</b> uncategorized
<b>Affected version:</b> git master	

#### Description

The Gauss transform classes as well as the density comparison classes operate on explicit float values where real values are desirable.

The reason for this is, that the reference data in all use-cases so far is explicitly float only, however we cannot guarantee that it will be like that for all the future use cases of these classes and thereby introduce an undesired precision loss in double precision versions of GROMACS.