GROMACS - Bug #16

Issue an error if pme_order < fourier_nx/y/z

10/03/2005 09:21 PM - Ramon Garcia

Status:	Closed		
Priority:	High		
Assignee:	Erik Lindahl		
Category:	mdrun		
Target version:	3.2.1		
Affected version - extra info:		**Difficulty:**	uncategorized
Affected version:			

Description

I found by a random test that if pme_order is less than the number of cells in a dimension of the Fourier grid Gromacs crashes. This is probably an invalid configuration (I know almost nothing about PME), but it is much better to issue an error in grompp than crashing.

Here is the code

in pme.c function make_bspline_moduli

```
650      for(i=0;i<nmax;i++)
651        bsp_data[i]=0;
652      for(i=1;i<=order;i++)
653        bsp_data[i]=data[i-1];
```

when order < nmax, the loop below access the array bsp_data beyond its bounds.

History

#1 - 10/03/2005 09:30 PM - Erik Lindahl

pme_order is always much smaller nx/ny/nz. Loop 1 zeros bsp_data[], and loop 2 copies the first order elements from data[].