**GROMACS - Bug #918**

**A possible bug to gmx_rdf.c**

04/13/2012 03:50 AM - Qikai Li

<table>
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<td>Priority:</td>
<td>Normal</td>
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<tr>
<td>Assignee:</td>
<td>Teemu Murtola</td>
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<td>Category:</td>
<td>analysis tools</td>
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<td>Target version:</td>
<td>4.5.6</td>
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**Description**

When I've checked the code on RDF / SF calculation, I found the following code segment may be problematic.

In file gmx_rdf.c:

```c
int i,j;
snew(t,x);  // <<====== bug ???
t = (t_complex *)calloc(x,sizeof(t_complex));
  if (!t) exit(fprintf(stderr,"allocation error");
t = (t_complex *)calloc(y,sizeof(t_complex));
  if (!t) exit(fprintf(stderr,"allocation error");
t[0] = (t_complex *)calloc(z,sizeof(t_complex));
  if (!t) exit(fprintf(stderr,"allocation error");

for (j = 1; j < y; j++)
  t[0][j] = t[0][j-1] + z;
for (i = 1; i < x; i++)
  {t[i] = t[i-1] + y;
   t[i][0] = t[i-1][0] + y*z;
    for (j = 1; j < y; j++)
     t[i][j] = t[i][j-1] + z;
   return t;
  }
```

**Associated revisions**

Revision 0a612e73 - 12/30/2012 07:35 AM - Teemu Murtola

Remove superfluous memory allocation.

The next line allocates the memory again.

Fixes #918.

Change-Id: i6f727cf059ccdc5d407b8398b9b29db625c120b8

**History**

#1 - 04/13/2012 02:56 PM - Szilárd Páll

- Category set to analysis tools

No offense, but there are quite a few issues with your report:

- that code is not in gmx_rdf.c, but in sfactor.c;
- we need some details why do you think the code is problematic, at first sight I don't see any problem;
- you should use "pre" formatting for code, otherwise it's impossible to read it.
#2 - 10/17/2012 10:26 PM - Roland Schulz
- Status changed from New to Feedback wanted

#3 - 12/30/2012 07:37 AM - Teemu Murtola
- Assignee set to Teemu Murtola
- Target version set to 4.5.6

The issue should be fixed by [https://gerrit.gromacs.org/#/c/1971/](https://gerrit.gromacs.org/#/c/1971/) (assuming this is what the original poster intended).

#4 - 12/31/2012 07:46 AM - Teemu Murtola
- Status changed from Feedback wanted to Closed