GROMACS - Bug #2711

Wrong Br and FE parameters in amber forcefields

10/26/2018 03:32 PM - Arthur Zalevsky

Status:	Closed		
Priority:	Normal		
Assignee:			
Category:			
Target version:			
Affected version - extra info:		**Difficulty:**	simple
Affected version:	2019-beta1		

Description

Br and FE are missing sigma and epsilon parameters defined in ffnonbonded.itp in amber forcefields.

Due to the formally defined parameters (bonded interactions seems valid though), systems passes grompp properly but usually explode after a short time.

```
amber03.ff/ffnonbonded.itp:Br           35       79.90     0.0000  A   0.00000e+00  0.00000e+00
amber03.ff/ffnonbonded.itp:FE           26       55.00     0.0000  A   0.00000e+00  0.00000e+00
amber94.ff/ffnonbonded.itp:Br           35       79.90     0.0000  A   0.00000e+00  0.00000e+00
amber94.ff/ffnonbonded.itp:FE           26       55.00     0.0000  A   0.00000e+00  0.00000e+00
amber96.ff/ffnonbonded.itp:Br           35       79.90     0.0000  A   0.00000e+00  0.00000e+00
amber96.ff/ffnonbonded.itp:FE           26       55.00     0.0000  A   0.00000e+00  0.00000e+00
amber99.ff/ffnonbonded.itp:Br           35       79.90     0.0000  A   0.00000e+00  0.00000e+00
amber99.ff/ffnonbonded.itp:FE           26       55.00     0.0000  A   0.00000e+00  0.00000e+00
amber99sb.ff/ffnonbonded.itp:Br           35       79.90     0.0000  A   0.00000e+00  0.00000e+00
amber99sb.ff/ffnonbonded.itp:FE           26       55.00     0.0000  A   0.00000e+00  0.00000e+00
amber99sb-ildn.ff/ffnonbonded.itp:Br          35       79.90     0.0000  A   0.00000e+00  0.00000e+0
0
amber99sb-ildn.ff/ffnonbonded.itp:FE          26       55.00     0.0000  A   0.00000e+00  0.00000e+0
0
amberGS.ff/ffnonbonded.itp:Br           35       79.90     0.0000  A   0.00000e+00  0.00000e+00
amberGS.ff/ffnonbonded.itp:FE           26       55.00     0.0000  A   0.00000e+00  0.00000e+00
```

Associated revisions

Revision cf9bd8e0 - 11/01/2018 08:31 AM - Paul Bauer

Properly define Bromine in amber forcefields

Added the proper values for Bromine to the amber forcefield definitions
in share/top/amber*/ffnonbonded.itp from the corresponding parm99.dat
file in amber itself.

Also removed the Iron parameters as they were not fully defined
and also not available in amber itself.

Fixes #2711

Change-Id: I8adb5dc1124ba39ab4a30568bd679a204dc83fc8

History

#1 - 10/27/2018 08:03 AM - Paul Bauer

Hello, do you have the corresponding parameters in the native amber forcefield description?
Also, can you give a sample system tpr that triggers the unexpected behaviour, so we can tell mdrun to be able to handle this kind of error as well?
Thanks!

#2 - 10/30/2018 09:38 AM - Arthur Zalevsky

- File br_zero.log added

- File br_zero.tpr added

- File br_fix.tpr added

Here's the part from original parm99.dat

```
  Br          2.22     0.320              Junmei(?)
```

and my values for parmbsc0(chi-OL3) (which is also based on amber99sb-ildn) according to acpype conversion formulas

```
[ atomtypes ]
;name      at.num   mass      charge ptype  sigma       epsilon
3 Br          35      79.90     0.0000  A   3.95559e-01  1.33888e+00 ; Converted from parm99.dat
```

tprs are in attach (sorry for them to be quite obsolete, but they were created several years ago for this project https://www.ncbi.nlm.nih.gov/pubmed/28717247)

#3 - 10/31/2018 09:57 AM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue #2711.
Uploader: Paul Bauer (paul.bauer.q@gmail.com)
Change-Id: gromacs~release-2018~I8adb5dc1124ba39ab4a30568bd679a204dc83fc8
Gerrit URL: https://gerrit.gromacs.org/8625

#4 - 11/01/2018 08:45 AM - Paul Bauer

- Status changed from New to Resolved

Applied in changeset cf9bd8e0287e50135bbe2e6246d8a7ece7c00f4c.

#5 - 11/01/2018 02:41 PM - Paul Bauer

- Status changed from Resolved to Closed

Files

br_zero.log	18.5 KB	10/30/2018	Arthur Zalevsky
br_zero.tpr	428 KB	10/30/2018	Arthur Zalevsky
br_fix.tpr	428 KB	10/30/2018	Arthur Zalevsky