GROMACS - Feature #2932
Failed to realloc error
04/25/2019 11:21 AM - Maxim Brodmerkel

Status: Closed
Priority: Normal
Assignee: mdrun
Category: mdrun
Target version: 2019.3
Difficulty: hard

Description
Hello,

I encountered an error while working on simulating the satellite tobacco necrosis virus, comprising 147960 atoms.

During the energy minimisation step using GROMACS version 2019.1 I encountered following error:

Fatal error:
Not enough memory. Failed to realloc 18446744065119617024 bytes for nlist->jjnr, nlist->jjnr=0x2b5cb01c9010

Or, after using 2016.6:

Fatal error:
Not enough memory. Failed to realloc -8589934592 bytes for nlist->jjnr, nlist->jjnr=3eb9a010

Further informations:
The simulations are done in the gas phase, with all-to-all neighbourlist and no cut-offs.

I hope you could help me with fixing this error.

With kind regards,
Maxim Brodmerkel

Associated revisions
Revision 5c4b41ed - 05/23/2019 10:09 AM - Paul Bauer
Add check for allocating too many interactions
Also change argument to nbxnn reallocation function from int to std::size_t to avoid signed integer overflow.
Fixes #2932
Change-Id: l97bdd825ba1e4d81b65b4e4c037f980164c571f2

History
#1 - 04/25/2019 12:38 PM - Berk Hess
- Status changed from New to Accepted
- Assignee deleted (Mark Abraham)
- Priority changed from High to Normal

You are not using a cut-off, so you are requesting interactions between all atoms pairs: (147960*2)/2 = 10^10 interactions. That is more than the maximum value of an int, so you get these weird errors. We should add a check for this. But even if this would work, is would be extremely slow. Use a cut-off, so you have a O(#atoms) instead of O(#atoms^2) computational problem.

It's probably not worth the effort to add a check for the group scheme, but we should add a check for the Verlet scheme, even if the issue occurs a (much) higher atoms counts there, because we use cluster pairs and we nearly always divide work over threads.
#2 - 05/21/2019 10:17 AM - Paul Bauer
- Status changed from Accepted to Fix uploaded
- Target version set to 2019.3

#3 - 05/23/2019 10:15 AM - Paul Bauer
- Status changed from Fix uploaded to Resolved

Applied in changeset 5c4b41ed47094d0bff2c04874a637c992ead885d.

#4 - 05/23/2019 03:22 PM - Paul Bauer
- Status changed from Resolved to Closed

## Files

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