GROMACS - Feature #2111

Implement Gaussian screening of electrostatics

02/01/2017 06:03 PM - David van der Spoel

Status:	In Progress	
Priority:	Normal	
Assignee:		
Category:		
Target version:		
Difficulty:	hard	

Description

It would be great to have the possibility of using screened interactions. A number of groups are working on this, e.g. http://pubs.acs.org/doi/abs/10.1021/ct5009069.

The main issue is that one extra parameter is needed per atom or atom type, which has to come from the topology in some way.

The Coulomb interaction would look like

V(r_ij) = q_i q_j erf(z_ij r_ij) / r_ij

History

#1 - 02/02/2017 02:37 PM - David van der Spoel

In the present form of the topology file each molecule could specify a new section with screening widths z_i. This in order to remain compatible to older topologies. E.g.:

[atom_properties]
; i type z_i^A z_i^B
1 1 10 12
2 1 8 6

In this way the format is ready for free energy calculations with changing z_i as well.
Since these lists would be generated normally this is not a big problem.

In order to get this into the tpr file we need to add this to the t_atoms structure, but for mdrun we need it in the mdatoms structure as well as the nbnxn_atomdata_t. That would mean minimal change to interfaces. However, a new tpr format would be needed.

#2 - 02/13/2017 10:43 AM - Berk Hess

Should the screening length be set be per atom or per atom type?
Note that some force fields, such as MCDHO, need it set per atom type pair. But I don't know if we want to support that.

#3 - 02/13/2017 01:00 PM - David van der Spoel

For flexibility it should be one screening length per atom I would say.
If we have one number per atom it should be possible to implement MCDHO shouldn't it?

#4 - 10/22/2017 02:01 PM - David van der Spoel

In order to make some progress we can start by patching topology reading and introduce a new section in top files that could look like this:
[distributed_charges]
; Atom Type Zeta ...
1 1 5.1
2 1 6.2

where type 1 would correspond to Gaussian with one zeta.

Other types could become more complex.

#5 - 10/22/2017 02:04 PM - David van der Spoel

The next step would be to update the SIMD kernels alternatively implement this in tables.

#6 - 11/05/2017 06:21 PM - Mohammad Ghahremanpour

David van der Spoel wrote:

The next step would be to update the SIMD kernels alternatively implement this in tables.

To use Gaussian charges, we only need the screening length, but for the Slater charges we also need to have the row number of the elements (atom) in the periodic table.
This can be determined based on the atomic number when filling the md_atoms. But, what if we want to change a Nitrogen to a Phosphor, for example, when moving the system from State A to State B. In this case, similar to mA and mB for mass, we need to have something like rowA and rowB. right?

#7 - 11/05/2017 06:34 PM - David van der Spoel

In that case we implement [distributed_charges] type 2.

#8 - 12/28/2017 08:52 AM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue #2111.
Uploader: David van der Spoel (spoel@xray.bmc.uu.se)
Change-Id: gromacs~master~I1ae5a38687b7ac65e3c2c51032c6e778b5c5d807
Gerrit URL: https://gerrit.gromacs.org/7396

#9 - 12/28/2017 03:00 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue #2111.
Uploader: David van der Spoel (spoel@xray.bmc.uu.se)
Change-Id: gromacs~master~I37cd2eea84fd24829adeb1d155775c0dbaeab57e
Gerrit URL: https://gerrit.gromacs.org/7398

#10 - 08/21/2018 08:46 AM - Gerrit Code Review Bot

Gerrit received a related DRAFT patchset '5' for Issue #2111.
Uploader: Natasha Kamerlin (natasha.kamerlin.gromacs@gmail.com)
Change-Id: gromacs~master~I5ed7e71ca85b73d703ae8e1d9c14b764e525f013
Gerrit URL: https://gerrit.gromacs.org/8200

#11 - 01/28/2019 08:36 PM - David van der Spoel

I would also like to implement free energy perturbation as soon as this one is incorporated into master. Will work out the equations.

#12 - 02/23/2019 10:31 AM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue #2111.
Uploader: David van der Spoel (spoel@xray.bmc.uu.se)
Change-Id: gromacs~master~I39ea11b63f2f5744ea114e9ac5533344526046d9
Gerrit URL: https://gerrit.gromacs.org/9216

#13 - 02/23/2019 12:33 PM - David van der Spoel

- Status changed from New to In Progress