# GROMACS - Feature #2451

## Linear virtual sites with fixed distance

03/14/2018 07:12 AM - David van der Spoel

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|---|---|---|
| **Status:** | Resolved | |
| **Priority:** | Normal | |
| **Assignee:** | David van der Spoel | |
| **Category:** | mdrun | |
| **Target version:** | | |
| **Difficulty:** | simple | |

**Description**

In the Charmm  force field linear virtual site are use for halogens to model halogen bonding. By design the distance between vsite particle and halogen atom is fixed at
CL-v: 0.016 nm,
BR-v: 0.019 nm, and
I-v: 0.022 nm

The present virtual_site2 does not support this since the position of the vsite is relative to two atoms and hence the distance can fluctuate. Here the proposal is make an additional virtual_site (type 2) with fixed distance to the halogen.

### Associated revisions

**Revision b766e6eb - 09/16/2019 12:47 PM - Berk Hess**

Add virtual site type 2FD

Fixes #2451

Change-Id: Ide9dcd829284567010435ed5cfb55194aed12dcf

### History

**#1 - 03/14/2018 09:08 AM - Berk Hess**

Is the vsite in between the two atoms or outside? Should we support both (using the sign of the distance)?

**#2 - 03/14/2018 09:19 AM - David van der Spoel**

Outside the halide atom I think, maybe Justin can comment, but this is a matter of definition for the implementation as well. I envision one could write
[ virtual_sites2 ]
; i  j  k type  distance
Vsite Cl  C 2  0.016

**#3 - 03/14/2018 11:35 AM - Justin Lemkul**

David van der Spoel wrote:

> Outside the halide atom I think, maybe Justin can comment, but this is a matter of definition for the implementation as well. I envision one could write
> [ virtual_sites2 ]
> ; i  j  k type  distance
> Vsite Cl  C 2  0.016

Yes, this is correct. In our convention, the construction is C-Cl-X. There could be other use cases, of course, and I agree that this could just be done with a sign convention (>0 for "outside" the bond, <0 for "inside").

**#4 - 03/14/2018 11:58 AM - Berk Hess**

I would think the consistent sign definition with the normal 2-atom vsite would be negative outside.

**#5 - 03/14/2018 02:05 PM - Justin Lemkul**

However we want to define it is fine, though it is a little confusing to have a negative number extend beyond the end of a bond. But I guess that's what documentation is for :)

**#6 - 03/14/2018 03:00 PM - Berk Hess**

A normal 2-atom vsite the parameter a, as one would expect, interpolates linear between atom i and j. So to get an atom sticking out from i you need a negative a.

#### #7 - 03/16/2018 09:46 PM - David van der Spoel

Just wondering whether fixing the 3FAD such that it can deal with 180 degree angles wouldn't be sufficient? It would do the trick for everything except diatomics like HF and CO.

#### #8 - 03/17/2018 04:35 PM - Justin Lemkul

David van der Spoel wrote:

> Just wondering whether fixing the 3FAD such that it can deal with 180 degree angles wouldn't be sufficient? It would do the trick for everything except diatomics like HF and CO.

From my perspective, 3fad would cover things. I'm not sure how many existing force fields will require this kind of construction for diatomics. I know CHARMM/CGenFF do not.

#### #9 - 03/19/2018 09:16 AM - Berk Hess

Looking at the manual I realized that you can already achieve what you want by using 3fd with j=k (and arbitrary a, e.g. a=0).
Implementing 2fd is then as simple as cut-and-pasting the 3fd code and removing k and a.
This also means that for consistency we should not have a minus sign for the "out" location.

#### #10 - 09/24/2018 11:02 PM - Mark Abraham

*- Status changed from New to Closed*

*- Target version deleted (2019)*

Sounds like there is a solution that doesn't need new GROMACS code.

#### #11 - 11/06/2018 06:34 PM - Justin Lemkul

To follow up on this issue, I have tried to do what Berk suggested with 3fd construction, and it indeed works just fine. The only issue is that grompp throws a warning about a duplicate atom number in the virtual site construction. That's fair, but should we add an exception, e.g. in the case of a=0, to allow for such odd behavior? I can get around this with -maxwarn 1, but I generally think doing so is poor practice and encourages users to ignore more significant issues.

#### #12 - 11/08/2018 04:10 AM - Justin Lemkul

Even worse, with version 2018, the virtual site construction throws an error that cannot be circumvented. I haven't tried the 2019 beta, but should I expect different behavior? This lone pair construction is essential for CGenFF going forward and our users are seeking solutions.

#### #13 - 11/08/2018 07:59 AM - David van der Spoel

Then let's get back to the original plan an implement a new type, 2fd. So we need a new type and a description here:

http://manual.gromacs.org/documentation/2019-beta2/reference-manual/functions/interaction-methods.html#virtual-interaction-sites

#### #14 - 09/12/2019 04:09 PM - Paul Bauer

*- Status changed from Closed to Accepted*

As stated this is an issue still and should be handled to allow CGenFF

#### #15 - 09/16/2019 01:15 PM - Berk Hess

*- Status changed from Accepted to Resolved*

Applied in changeset b766e6ebfa539173b4b3580ca5356533a27a8caa.