

## GROMACS - Task #1876

### Reorganize vector input passed to core MD routines

12/11/2015 03:26 PM - Berk Hess

|                        |               |
|------------------------|---------------|
| <b>Status:</b>         | New           |
| <b>Priority:</b>       | Normal        |
| <b>Assignee:</b>       |               |
| <b>Category:</b>       | core library  |
| <b>Target version:</b> | future        |
| <b>Difficulty:</b>     | uncategorized |

#### Description

The core MD routines need to be fast and many are currently being converted to use SIMD intrinsics. This means that the inputs (x, v, f, ?) need to be SIMD aligned, sometimes padded at the end. A peculiar, currently relevant, issue is that we need one element extra for unaligned 4-wide SIMD loads (which is not the same as padded up to a multiple of the SIMD width!), see: <https://gerrit.gromacs.org/#/c/5445/>

To ensure these requirements, we need ways to check that the input to core MD routines have alignment and paddings. This probably means we can't pass plain rvecs to thing like `do_force()` or `constrain()`. I guess the proper way is to define an MD rvec object with its own allocator.

#### History

##### #1 - 12/13/2015 01:18 PM - Erik Lindahl

This problem should already be solved: Use STL containers with the `AlignedAllocator` we already have in the code.

##### #2 - 06/01/2016 01:59 PM - Mark Abraham

- Target version changed from 2016 to future