Masses are incorrectly evaluated for certain types of dynamic selections

For dynamic selections that compute center-of-mass or center-of-geometry positions of more than one atom, the total mass and charge are incorrectly calculated if the set of atoms changes between frames. For example, the following selection can cause issues:

```
res_com of (y > 2)
```

The masses are reported for all frames as they were on the initial evaluation, i.e., in this case for the whole residue. They may be too big if not all atoms of the residue are selected by the y > 2 condition for some particular frame.

Does not affect the behavior of `g_select` in 4.5 or 4.6, and is a relatively rare use case, so targeting the fix for 5.0 only.

Associated revisions

**Revision 9edd19d5 - 02/13/2013 10:27 PM - Teemu Murtola**

Add tests for selection mass evaluation and fix it.

Removed unnecessary and at times incorrect precalculation of total masses and charges for selected positions. Evaluate them again for each frame if they may have changed.

Noticed when adding some tests for this behavior; the tests are also added here.

Also store the masses and charges again in continuous arrays in preparation for exposing those arrays.

Fixes #1145.

Change-Id: Ifa23d042706d9f2a0b8aa142338812f055f6f60a

History

#1 - 02/08/2013 02:28 PM - Teemu Murtola
   - Status changed from New to In Progress

#2 - 02/16/2013 06:35 AM - Teemu Murtola
   - Status changed from In Progress to Closed

#3 - 07/17/2013 07:16 AM - Teemu Murtola
   - Category changed from analysis tools to selections
   - Affected version set to 5.0