Corrections to: All-atom computations with irreversible Markov chains[1]

(Dated: 4 October 2018)

In the following, we collect misprints and ambiguous wordings in the published article[1]. They are also present in the preprint arXiv:1804.05795V1 (16 April 2018). They will be corrected in upcoming versions on arXiv.

1. In the line just before eq. (23), the words "lifting variable describing which particle is 'active"' should be replaced by "lifting variable describing that particle a is 'active"'.

2. Right below eq. (53), the sequence of three outcomes ("First"..., "Second" ..., "Third"...) is inconsistent with the sequence "A", "B", and "C" in Fig. 4b. For added clarity, the sequence of three outcomes should be rearranged. The "First" outcome (case "A" in Fig. 4b) should be a cell event that is not confirmed as a particle event. The "Second" outcome (case "B" in Fig. 4b) should be a cell event that is confirmed as a particle event. The "Third" outcome (case "C" in Fig. 4b) should be a cell-boundary event.

3. For added clarity, in the 11th line below eq. (53), "$q_{M,1}(\mathbf{r}_1, \mathbf{r}_2)$" should be changed to "$q_{M,1}(\mathbf{r}_1 + \eta\hat{\mathbf{e}}_x, \mathbf{r}_2)$".

4. There is a mistake in Eq. (63). It should read:

$$\tilde{q}_{(\{1,2\},\,\mathrm{Coulomb}_{\mathbf{n}}),1}(\mathbf{r}_{12}) = c_1 c_2 \left\{ \frac{x_{12} + n_x L}{|\mathbf{r}_{12} + \mathbf{n}L|^3} + \frac{1}{pL}\left[\frac{1}{|\mathbf{r}_{12} + L\,(\mathbf{n} + p\hat{\mathbf{e}}_x/2)\,|} - \frac{1}{|\mathbf{r}_{12} + L\,(\mathbf{n} - p\hat{\mathbf{e}}_x/2)\,|} \right] \right\}. \tag{63}$$

   The correct formula was used in all the explicit computations.

5. Eq. (99) should read:

$$U_{(\{i,j\},\,\mathrm{rep})}(\mathbf{r}_{ij}) = k_2 \left(\frac{r_0}{|\mathbf{r}_{ij}|} \right)^6. \tag{99}$$

   This is the version that was used in all the explicit computations.

ACKNOWLEDGMENTS

We thank Philipp Höllmer and Seiji Miyashita for pointing out some of these misprints and imprecisions.

[1] M. F. Faulkner, L. Qin, A. C. Maggs, and W. Krauth, The Journal of Chemical Physics **149**, 064113 (2018).