CORRECTION

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Correction: Generalized Langevin dynamics: construction and numerical integration of non-Markovian particle-based models

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Correction for 'Generalized Langevin dynamics: construction and numerical integration of non-Markovian particle-based models' by Gerhard Jung *et al.*, *Soft Matter*, 2018, DOI: 10.1039/c8sm01817k.

Algorithm 1 presented in the manuscript on page 4 contains a significant typographical error which was introduced in the typesetting process. Line 13 of Algorithm 1 in the published manuscript is: $x^{k+1} = \left\| \hat{W}_\omega \right\|^{k+1} \sqrt{H^{k+1}} e^0$ and has been corrected to $x^{k+1} = \left\| \hat{W}_\omega \right\| V^{k+1} \sqrt{H^{k+1}} e^0$. The full and correct algorithm is repeated below.

Algorithm 1: Generating correlated random numbers $F_{I,n}$ with the distribution $\langle F_{I,n+m} F_{J,n} \rangle = K_{IJ,m}$

1: **Inputs:**

$K_{IJ,m}$ for $m = 0, \ldots, m_{\max} - 1$ with $K_{IJ,m} = K_{IJ,-m}$

$W_{I,n}$ with $\langle W_{I,n+m} W_{J,n} \rangle = \delta_{m0} \delta_{IJ}$

2: **Initialize:**

$$\text{compute } \hat{K}_{IJ,\omega} = \sum_{m=-m_{\max}+1}^{m_{\max}-1} K_{IJ,m} \exp\left(-\mathrm{i} m \omega \frac{2\pi}{2m_{\max} - 1} \right)$$

$$\text{compute } \hat{W}_{I,\omega} = \sum_{m=-m_{\max}+1}^{m_{\max}-1} W_{I,n+m} \exp\left(-\mathrm{i} m \omega \frac{2\pi}{2m_{\max} - 1} \right)$$

3: **for** $\omega = 0$ to $m_{\max} - 1$ **do**

4:      set $v_I^0 = 0$, $\beta^0 = 0$, $v_I^1 = \hat{W}_{I,\omega} / \|\hat{W}_\omega\|$, $k = 1$, $\Delta = 1$

5:      compute $\alpha^1 = v_I^1 \hat{K}_{IJ,\omega} v_J^1$

6:      **while** $\Delta > tol$ **do**

7:          compute $r_I^{k+1} = \hat{K}_{IJ,\omega} v_J^k - \alpha^k v_I^k - \beta^{k-1} v_I^{k-1}$

8:          set $\beta^k = \|r^{k+1}\|$

9:          set $v_I^{k+1} = r_I^{k+1} / \beta^k$

10:         compute $\alpha^{k+1} = v_I^{k+1} \hat{K}_{IJ,\omega} v_J^{k+1}$

11:         define $V_{Ip}^{k+1} = v_I^p$, $p = 1, \ldots, k+1$

12:         construct tridiagonal H_{pq}^{k+1} with diagonal elements equal to $(\alpha_1, \ldots, \alpha_{k+1})$ and super- and sub-diagonal elements equal to $(\beta_1, \ldots, \beta_k)$

13:         compute $x^{k+1} = \left\| \hat{W}_\omega \right\| V^{k+1} \sqrt{H^{k+1}} e^0$, with $e_1^0 = 1$ and $e_q^0 = 0$, $q = 2, \ldots, k+1$

14:         set $\Delta = \|x^{k+1} - x^k\|$

15:         set $k = k + 1$

16:      **end while**

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17:     set $\hat{F}_{I,\omega} = x_I^k$

18: **end for**

19: compute $F_{I,n} = \dfrac{1}{m_{\max}} \left(\hat{F}_{I,0} + 2 \displaystyle\sum_{\omega=1}^{m_{\max}-1} \hat{F}_{I,\omega} \right)$

The Royal Society of Chemistry apologises for these errors and any consequent inconvenience to authors and readers.