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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: $\boldsymbol{x}^{k+1} = \left\|\hat{\boldsymbol{W}}_\omega\right\|^{k+1}\sqrt{\boldsymbol{H}^{k+1}}\boldsymbol{e}^0$ and has been corrected to $\boldsymbol{x}^{k+1} = \left\|\hat{\boldsymbol{W}}_\omega\right\|\boldsymbol{V}^{k+1}\sqrt{\boldsymbol{H}^{k+1}}\boldsymbol{e}^0$. 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:**

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

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

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 $\beta^k = \|\boldsymbol{r}^{k+1}\|$

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

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

15: set $k = k + 1$

16: **end while**

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set $\hat{F}_{I,\omega} = x_I^k$
end for
compute $F_{I,n} = \frac{1}{m_{\max}}\left(\hat{F}_{I,0} + 2\sum_{\omega=1}^{m_{\max}-1}\hat{F}_{I,\omega}\right)$

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