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

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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:  $\mathbf{x}^{k+1} = \|\hat{\mathbf{W}}_\omega\|^{k+1} \sqrt{\mathbf{H}^{k+1}} \mathbf{e}^0$  and has been corrected to  $\mathbf{x}^{k+1} = \|\hat{\mathbf{W}}_\omega\| \mathbf{v}^{k+1} \sqrt{\mathbf{H}^{k+1}} \mathbf{e}^0$ . 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  $m = 0, \dots, m_{\max} - 1$  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  $\hat{K}_{IJ,\omega} = \sum_{m=-m_{\max}+1}^{m_{\max}-1} K_{IJ,m} \exp\left(-im\omega \frac{2\pi}{2m_{\max}-1}\right)$   
 compute  $\hat{W}_{I,\omega} = \sum_{m=-m_{\max}+1}^{m_{\max}-1} W_{I,n+m} \exp\left(-im\omega \frac{2\pi}{2m_{\max}-1}\right)$

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

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

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

**6: while**  $\Delta > \text{tol}$  **do**

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

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

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

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

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

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

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

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

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

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

