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A new class of highly efficient exact stochastic simulation algorithms for chemical reaction networks

Notes and Corrections

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I. Corrections

- A typo in the published version of the PDM algorithm (Table 1 of the published article) has been fixed. A prime was missing in the reaction index in steps 5.2.2 and 5.2.3. The corrected algorithm can be found on Page 2 of this document. We thank Jonathan Blakes and Daven Sanassy (both from the University of Nottingham, UK) for reporting this typo.

II. Notes

- The population of the reservoir (source) in source reactions should be set to 1 with a corresponding stoichiometry of 0. This will ensure that one doesn't divide by zero in Eq. 4 of the published article.

1. Initialization: set $t \leftarrow 0$; initialize $\mathbf{n}$, $\mathbf{\Pi}$, $\mathbf{\Lambda}$, $\mathbf{\Sigma}$; $a \leftarrow \sum_{i=0}^{N} \Sigma_i$; $\Delta a \leftarrow 0$; generate $\mathbf{L}$, $\mathbf{U}^{(1)}$, $\mathbf{U}^{(2)}$, and $\mathbf{U}^{(3)}$

2. Sample μ: generate a uniform random number $r_1 \in [0, 1)$ and determine the group index I and the element index J according to Eqs. (2), (4), and (5); $\mu \leftarrow \mathrm{L}_{I,J}$

3. Sample τ: generate a uniform random number $r_2 \in [0, 1)$ and compute the time to next reaction τ as $\tau \leftarrow a^{-1} \ln(r_2^{-1})$

4. Update $\mathbf{n}$: for each index k of $\mathbf{U}_{\mu}^{(1)}$, $l \leftarrow \mathrm{U}_{\mu,k}^{(1)}$ and $n_l \leftarrow n_l + \mathrm{U}_{\mu,k}^{(2)}$

5. Update $\mathbf{\Pi}$, $\mathbf{\Lambda}$, $\mathbf{\Sigma}$ and compute Δa, the change in a:

   For each index k of $\mathbf{U}_{\mu}^{(1)}$, do:

   5.1. $l \leftarrow \mathrm{U}_{\mu,k}^{(1)}$

   5.2. For each index m of $\mathbf{U}_{l}^{(3)}$, do:

      5.2.1. $(i_m^l,\, j_m^l) \leftarrow \mathrm{U}_{l,m}^{(3)}$ (Eq. 6)

      5.2.2. **(Corrected)** $\Pi_{i_m^l, j_m^l} \leftarrow \Pi_{i_m^l, j_m^l} + c_{\mu'} \mathrm{U}_{\mu,k}^{(2)}$, $\mu' = \mathrm{L}_{i_m^l, j_m^l}$ if $l \neq i_m^l$

      (Corrected) $\Pi_{i_m^l, j_m^l} \leftarrow \Pi_{i_m^l, j_m^l} + \frac{1}{2} c_{\mu'} \mathrm{U}_{\mu,k}^{(2)}$, $\mu' = \mathrm{L}_{i_m^l, j_m^l}$ if $l = i_m^l$

      5.2.3. **(Corrected)** $\Lambda_{i_m^l} \leftarrow \Lambda_{i_m^l} + c_{\mu'} \mathrm{U}_{\mu,k}^{(2)}$, $\mu' = \mathrm{L}_{i_m^l, j_m^l}$ if $l \neq i_m^l$

      (Corrected) $\Lambda_{i_m^l} \leftarrow \Lambda_{i_m^l} + \frac{1}{2} c_{\mu'} \mathrm{U}_{\mu,k}^{(2)}$, $\mu' = \mathrm{L}_{i_m^l, j_m^l}$ if $l = i_m^l$

      5.2.4. $\Sigma_{\mathrm{temp}} \leftarrow \Sigma_{i_m^l}$

      5.2.5. $\Sigma_{i_m^l} \leftarrow n_{i_m^l} \Lambda_{i_m^l}$

      5.2.6. $\Delta a \leftarrow \Delta a + \Sigma_{i_m^l} - \Sigma_{\mathrm{temp}}$

   5.3. $\Delta a \leftarrow \Delta a + n_l \Lambda_l - \Sigma_l$; $\Sigma_l \leftarrow n_l \Lambda_l$

6. Update a and increment time: $a \leftarrow a + \Delta a$; $\Delta a \leftarrow 0$; $t \leftarrow t + \tau$

7. Go to step 2

Table 1: Detailed algorithm for the partial-propensity direct method PDM.