

Efficient simulation of stochastic chemical kinetics with the Stochastic Bulirsch-Stoer extrapolation method: Supplementary information

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In this file we show the plots for error versus runtime for all the species of the chain decay, Michaelis-Menten, Schlögl and mutually inhibiting enzymes systems.

Chain decay system

Fig. A1 shows histogram errors for all species from 5×10^5 SBS, SBS-DA, TL, TTTL and UBTL simulations. The SBS safety factors are $S_1 = 0.2, S_2 = 0.4$, those for the SBS-DA are $S_1 = 0.15, S_2 = 0.2, a_{tol} = 10^{-6}$, and error parameters corresponding to each point (going left to right) are listed in Table 3 of the article. TTTL parameter $\theta = 0.55$.

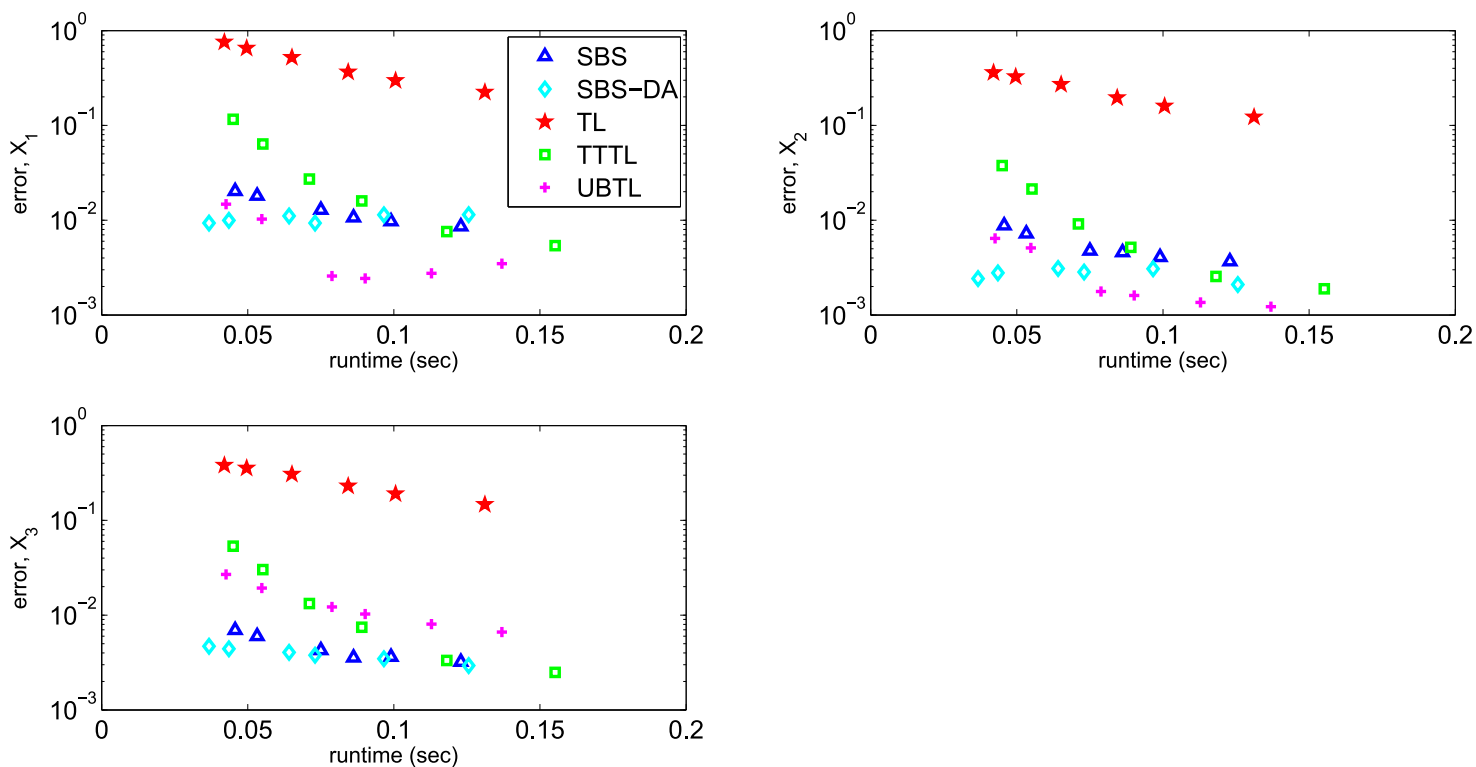


Figure A1: **Chain decay system efficiency for all species and all methods.** Histogram errors of all three species versus time for a single simulation.

Michaelis-Menten system

Fig. A2 shows histogram errors for all species from 10^6 SBS, SBS-DA, TL, TTTL and UBTL simulations. The SBS safety factors are $S_1 = S_2 = 0.35$, and those of the SBS-DA are $S_1 = S_2 = 0.33$, $a_{tol} = 10^{-6}$, and error parameters corresponding to each point (going left to right) are listed in Table 3 of the article. TTTL parameter $\theta = 0.55$.

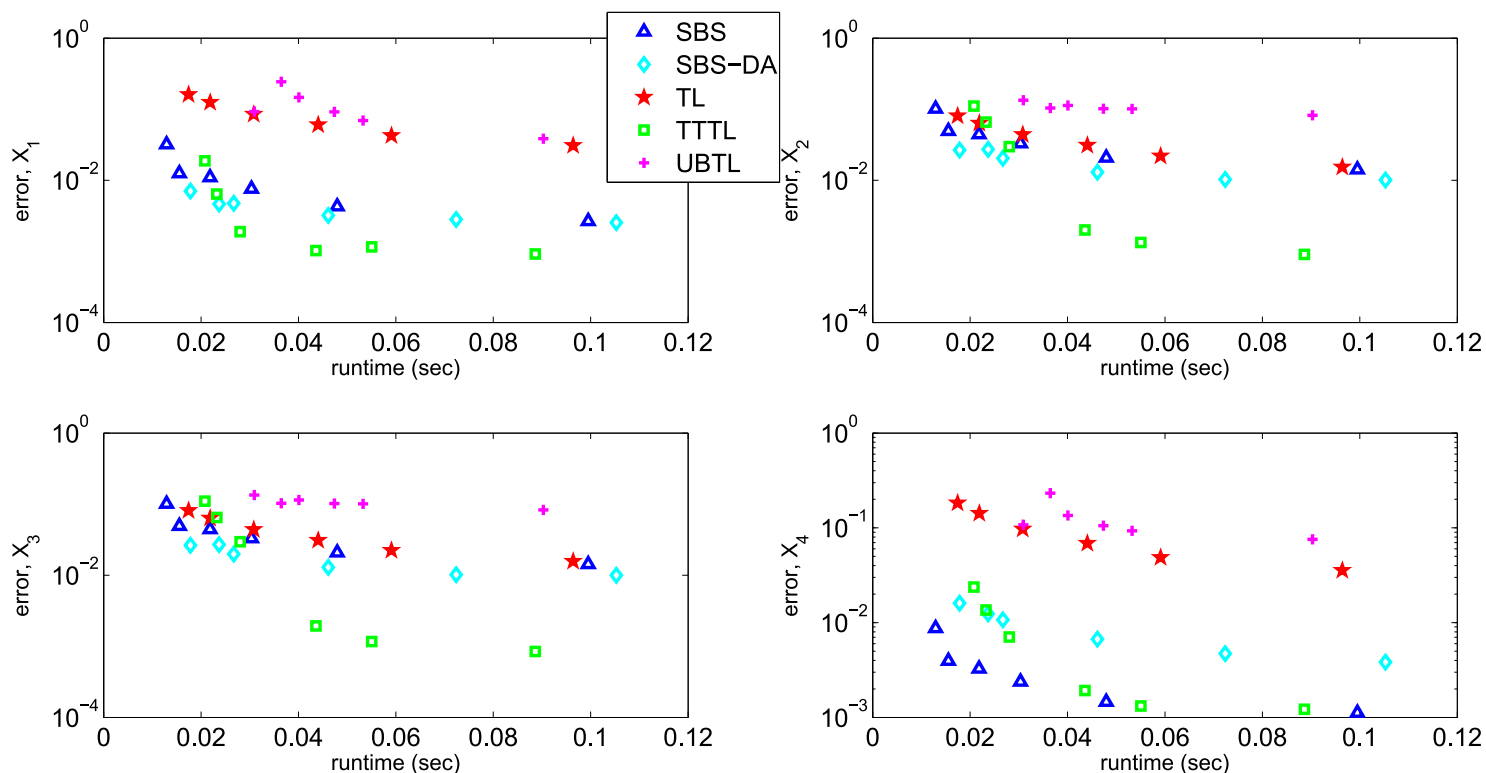


Figure A2: **Michaelis-Menten system efficiency for all species and all methods.** Histogram errors of all four species versus time for a single simulation.

Schlögl system

Fig. A3 shows histogram errors for all species from 2×10^5 SBS, SBS-DA, TL, TTTL and UBTL simulations. The SBS safety factors are $S_1 = S_2 = 0.05$, those for the SBS-DA are $S_1 = S_2 = 0.125$, $a_{tol} = 10^{-6}$, and error parameters corresponding to each point (going left to right) are listed in Table 3 of the article. TTTL parameter $\theta = 0.55$.

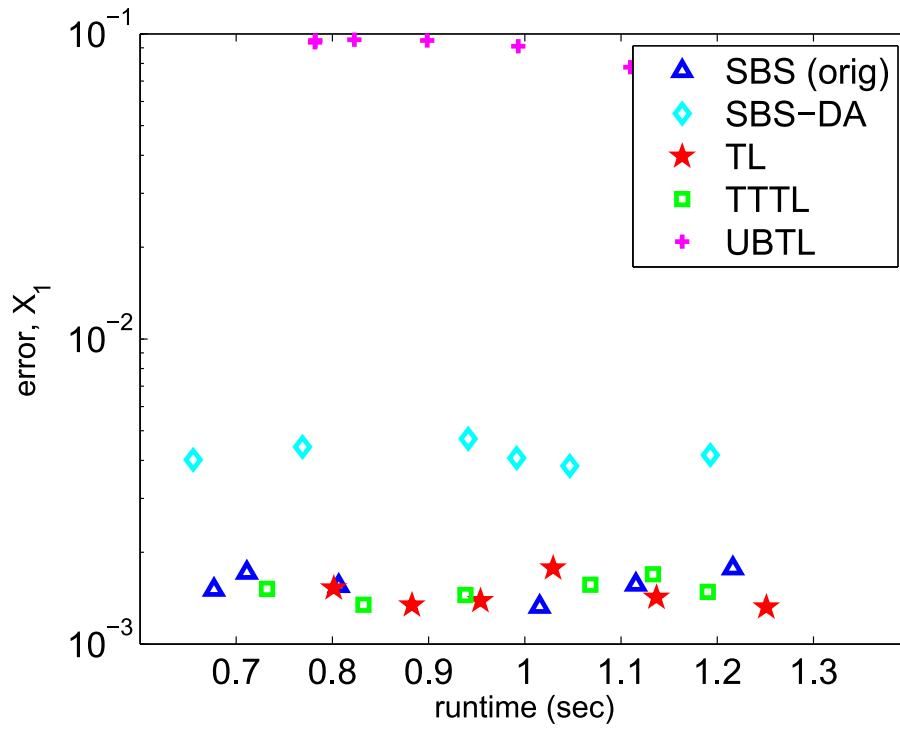


Figure A3: **Schlögl system efficiency for the only species and all methods.** Histogram errors of all four species versus time for a single simulation.

Mutually inhibiting enzymes system

Fig. A4 shows histogram errors for all species from 2×10^5 SBS, TL, TTTL and UBTL simulations. The SBS safety factors are $S_1 = S_2 = 0.4$ and $S_1 = 0.55, S_2 = 0.7$ for the SBS-DA, with $a_{tol} = 10^{-6}$, and error parameters corresponding to each point (going left to right) are listed in Table 3 of the main text. TTTL parameter $\theta = 0.55$.

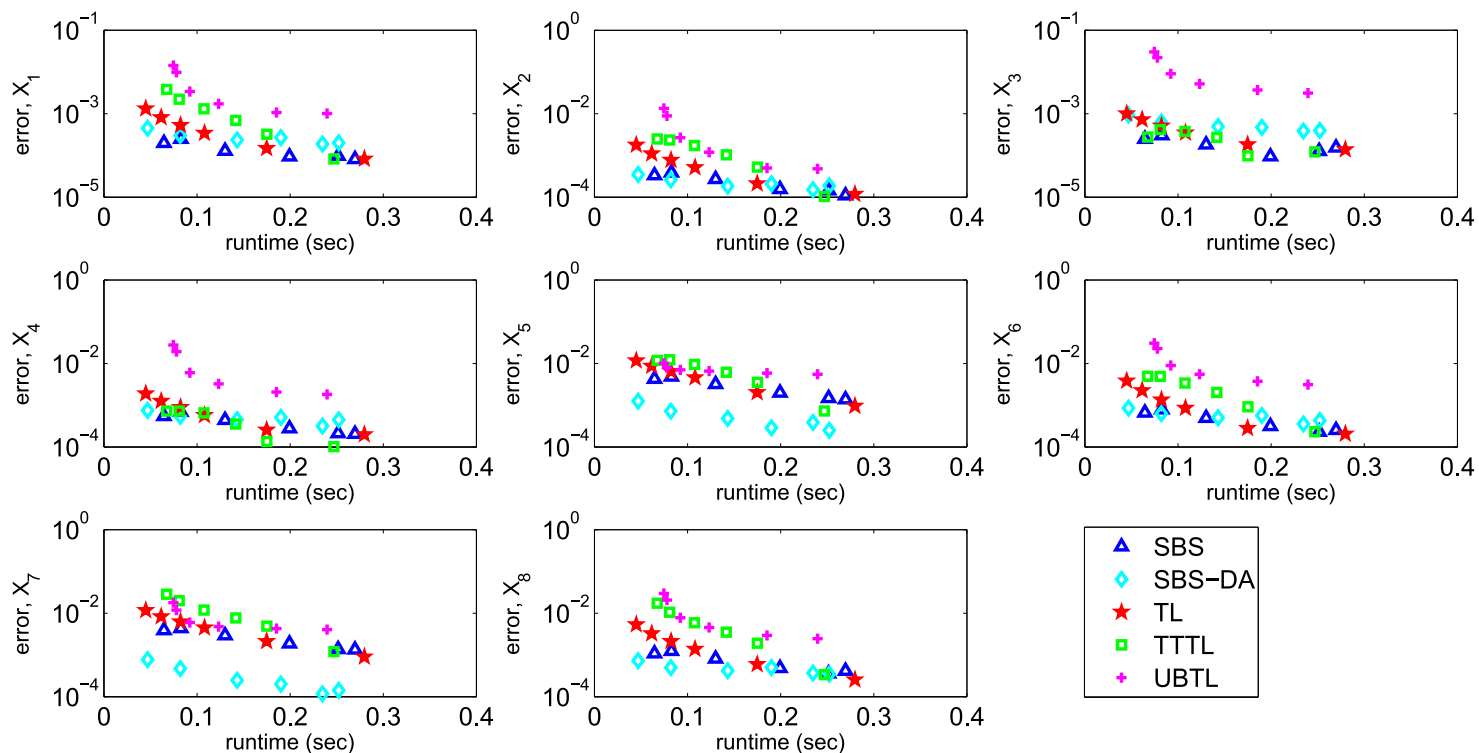


Figure A4: **Mutually inhibiting enzymes system efficiency for all species and all methods.** Histogram errors of all eight species versus time for a single simulation.