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 $5 \times 10^5$ 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 $S_1 = 0.15, S_2 = 0.2, a_{tot} = 10^{-6}$, 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.](image)

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 $S_1 = S_2 = 0.33$, $a_{tot} = 10^{-6}$, 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 $2 \times 10^5$ 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 $S_1 = S_2 = 0.125, a_{tot} = 10^{-6}$, 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: Schlossgl system efficiency for the only species and all methods.](image)

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 $2 \times 10^5$ 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.](image-url)