Supplementary File S3: Determining an error bound for the Hybrid τ-leaping simulation model

A reasonable choice of the error bound ϵ $(0 < \epsilon \ll 1)$ for the hybrid τ-leaping simulation model was further investigated by exploring the trade-off between simulation accuracy and computational speed at some fixed parameter values (Table 1) based on 100 different simulation realisations or repetitions; where each simulation realisation corresponded to the nine observed parasite-fish groups (given fish sex, fish size, fish stock and parasite strain). The simulation accuracy was quantified by the mean square error (given by equation 1) based on the mean (simulated) parasite numbers over time (day 1 to 17) from the exact SSA (Algorithm 5) and the hybrid τ-leaping algorithm (Algorithm 6) at 10 different error bound values ($\epsilon = 0.002, 0.004, 0.006, 0.008, 0.01, 0.02, 0.04, 0.06, 0.08$ and 0.1); such that

$$\mathrm{MSE}\left(\bar{X}^{(g)}_{\mathrm{leap}}(t), \bar{X}^{(g)}_{\mathrm{SSA}}(t)\right) = \frac{1}{100}\sum_{r=1}^{100}\left(\bar{X}^{(g)}_{\mathrm{leap},r}(t) - \bar{X}^{(g)}_{\mathrm{SSA},r}(t)\right)^2, \tag{1}$$

where $\bar{X}^{(g)}_{\mathrm{leap},r}(t)$ and $\bar{X}^{(g)}_{\mathrm{SSA},r}(t)$ are the mean parasite numbers over time t from hybrid $\tau - leaping$ and exact SSA, respectively; across each of the nine parasite-fish groups (g) and simulation realisation (r). The respective confidence intervals of the mean over time between the two simulation methods were also compared at $0 < \epsilon < 0.1$ for each parasite-fish group over time. The simulation speed was quantified by the computational time (computer's CPU time measured in seconds).

It was discovered that the simulation accuracy reduces in the hybrid τ-leaping algorithm as the error bound (ϵ) increases from $\epsilon = 0.002$ to $\epsilon = 0.1$ (see Figure 1). From Figures 6.4-6.13, it can be observed that the mean parasite numbers from the hybrid τ-leaping simulations were relatively consistent with the exact SSA at error bounds, $0.002 \leq \epsilon \leq 0.01$, across the nine parasite-fish groups (see Figures 2–6); including their respective confidence intervals. At $\epsilon \geq 0.02$, the τ-leaping algorithm started to perform badly across the parasite-fish groups as the error bound increased towards $\epsilon = 0.1$ (see Figures 7–11). Figure 12 shows that at $\epsilon = 0.008$ or $\epsilon = 0.01$, the τ-leaping algorithm was relatively fast but not very significant from the computational time of the exact SSA. This may be due to either the smaller number of simulation repetitions (100 repetitions) or the number of parasites from the simulations being relatively small over time at the pre-specified parameter values (which were randomly chosen). Thus, the leaping condition was not met most of the time for just these simple explorations. However, it has already been shown in the Supplementary File S1 concerning the B-D-C process that once the leap condition is met, τ-leaping is much faster compared to the exact SSA (otherwise, the latter is used the proposed hybrid $\tau-$leaping algorithm given by Algorithm 6). Based on the simulation accuracy and computational speed, $\epsilon = 0.01$ can be a reasonable choice of the error bound for subsequent simulations from the multidimensional stochastic model.

Table 1: Fixed parameter values for choosing an error bound

Parameters	Fixed values
Base simulation parameters	
b_{11}	0.668
b_{12}	0.018
b_{21}	0.668
b_{22}	0.018
b_{31}	0.668
b_{32}	0.018
d_{11}	0.008
d_{12}	0.071
d_{21}	0.008
d_{22}	0.071
d_{31}	0.008
d_{32}	0.071
m	0.083
r	0.001
s	0.009
κ	182
Additional simulation parameters	
ϵ_1	0.545
ϵ_2	0.333
ϵ_3	0.001
r_1	0.351
r_2	0.196
r_3	0.994
s_1	0.041

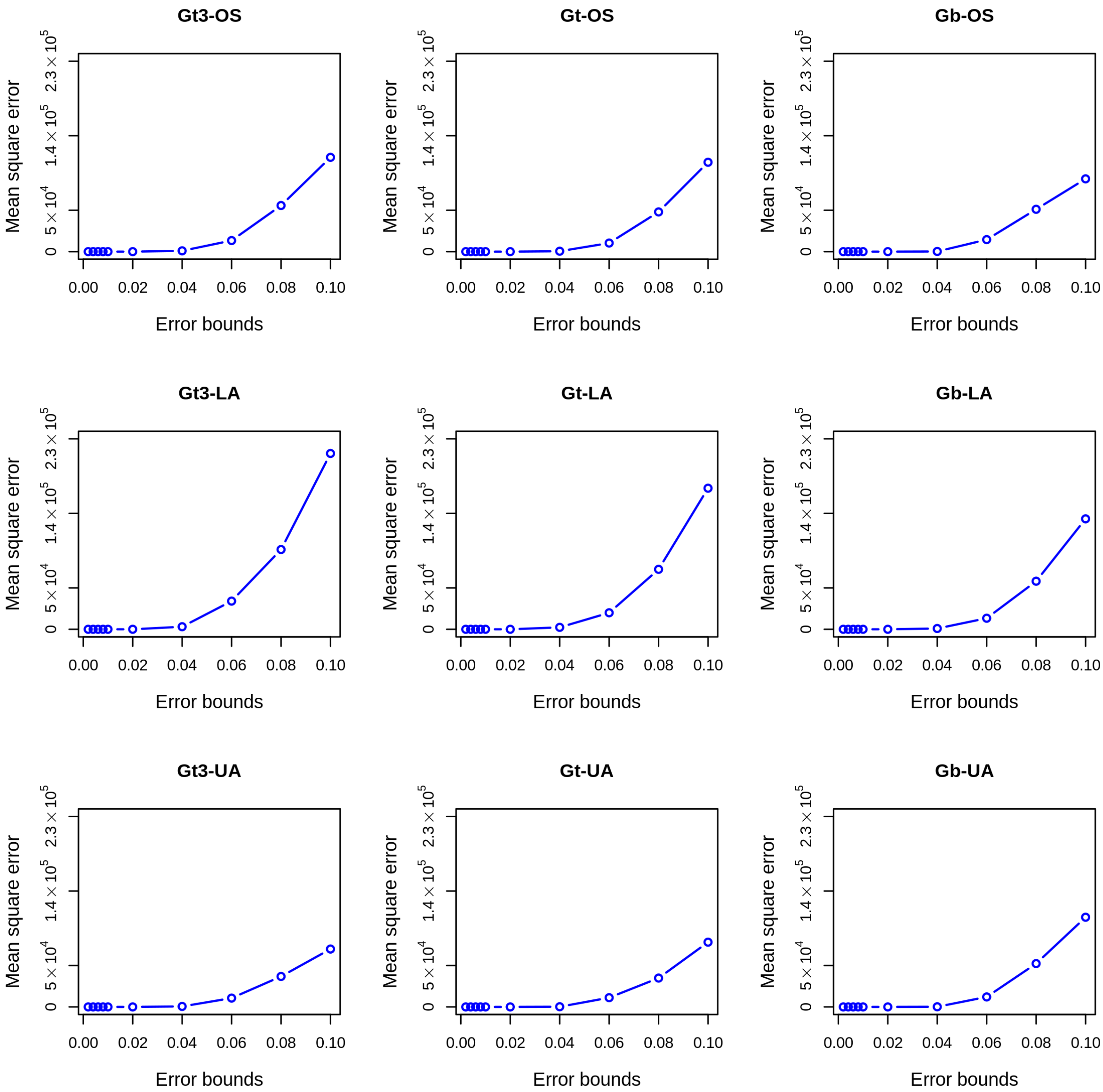

Figure 1: Mean square error from the Hybrid τ-leaping algorithm at different error bounds.

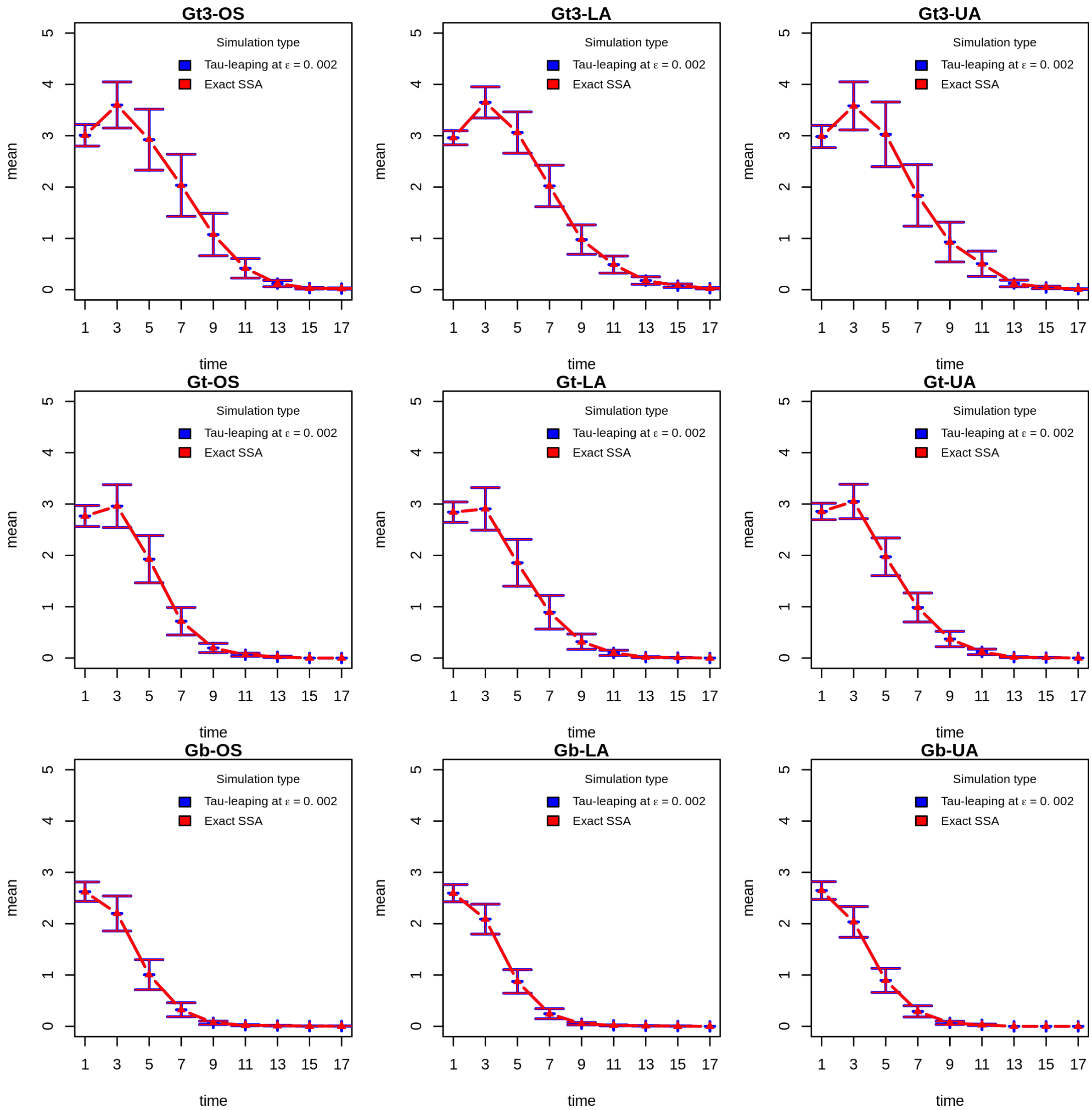

Figure 2: Mean comparison between exact SSA and Hybrid τ-leaping simulations at $\epsilon = 0.002$.

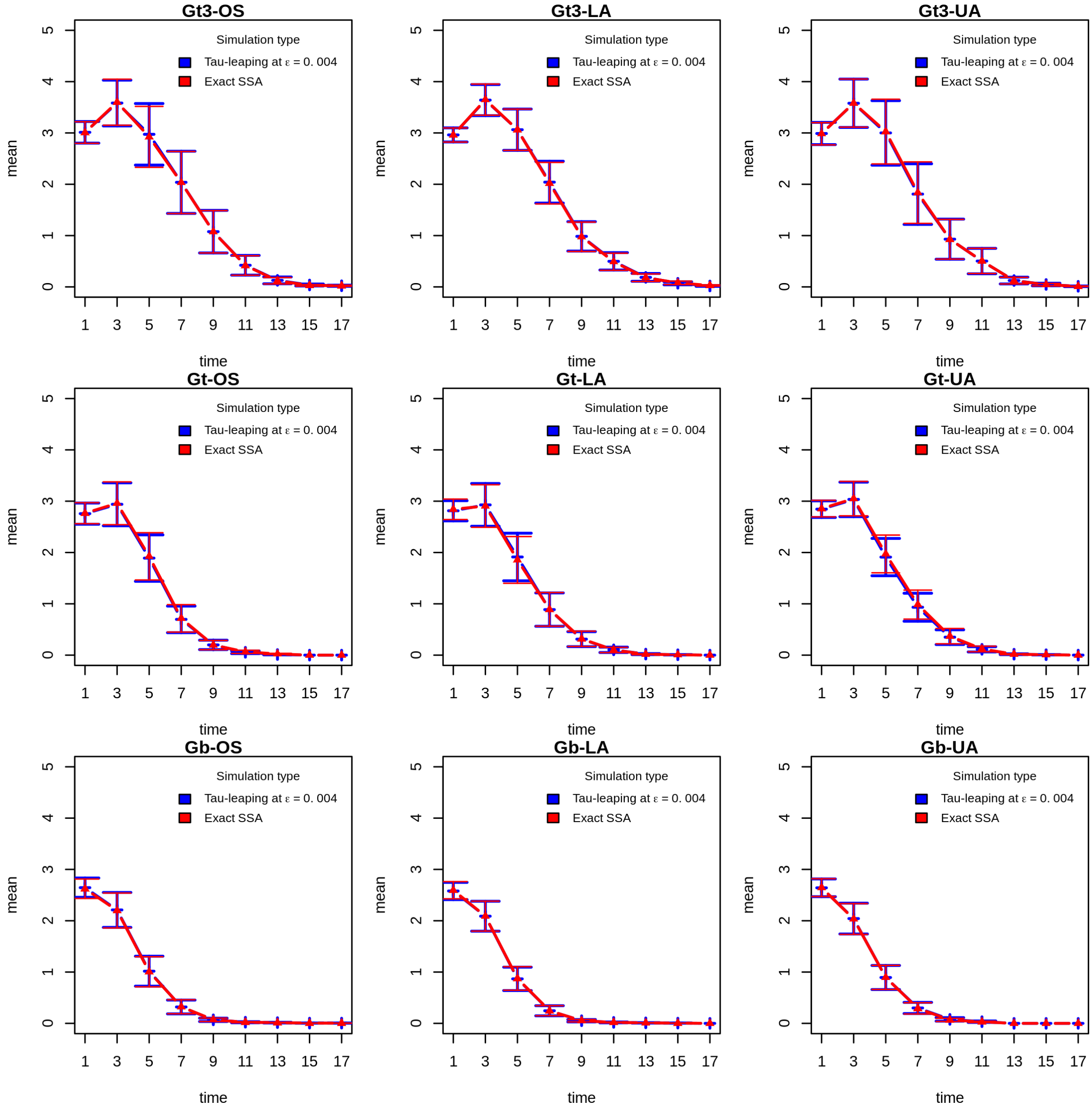

Figure 3: Mean comparison between exact SSA and Hybrid τ-leaping simulations at $\epsilon = 0.004$.

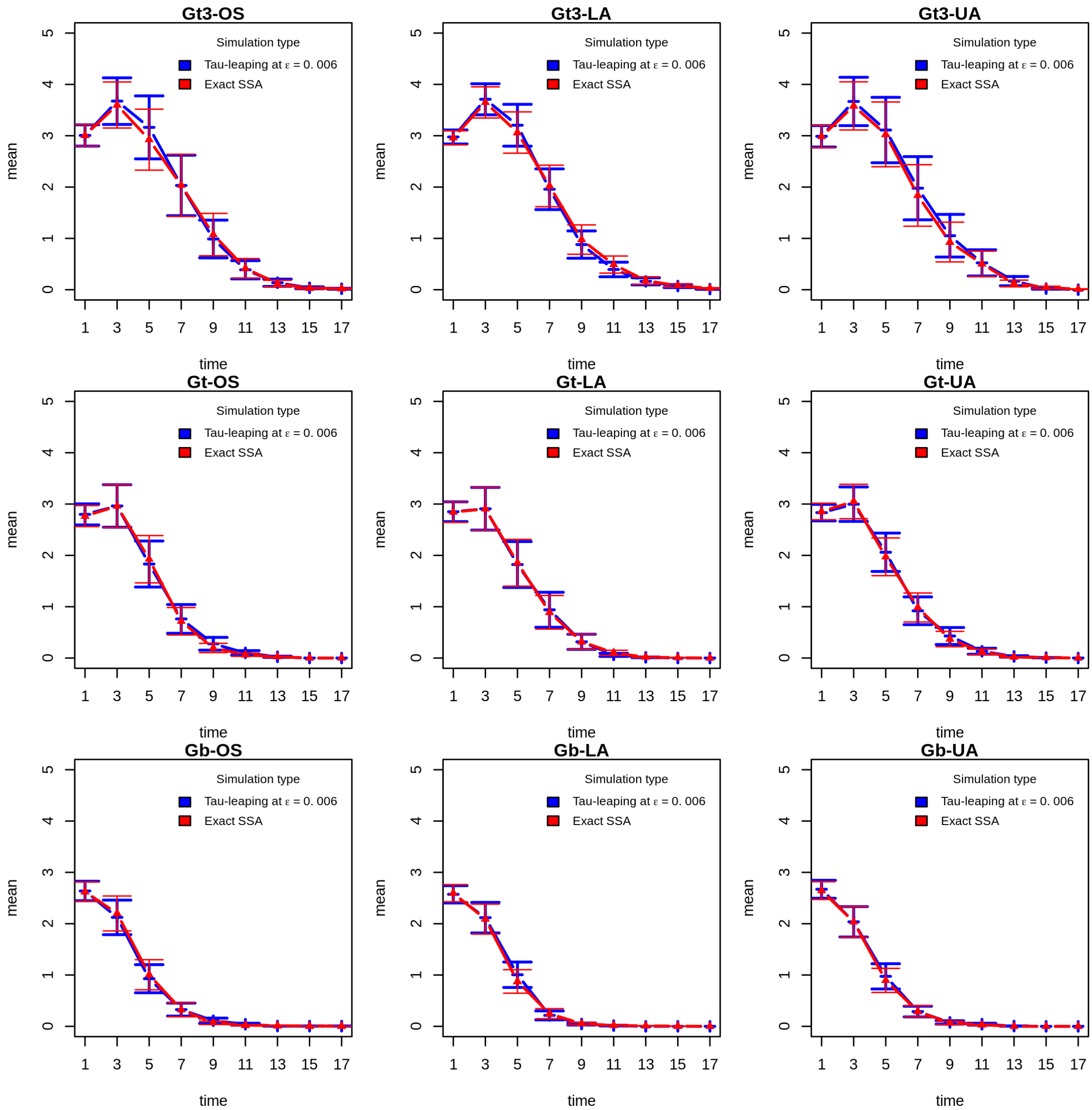

Figure 4: Mean comparison between exact SSA and Hybrid τ-leaping simulations at $\epsilon = 0.006$.

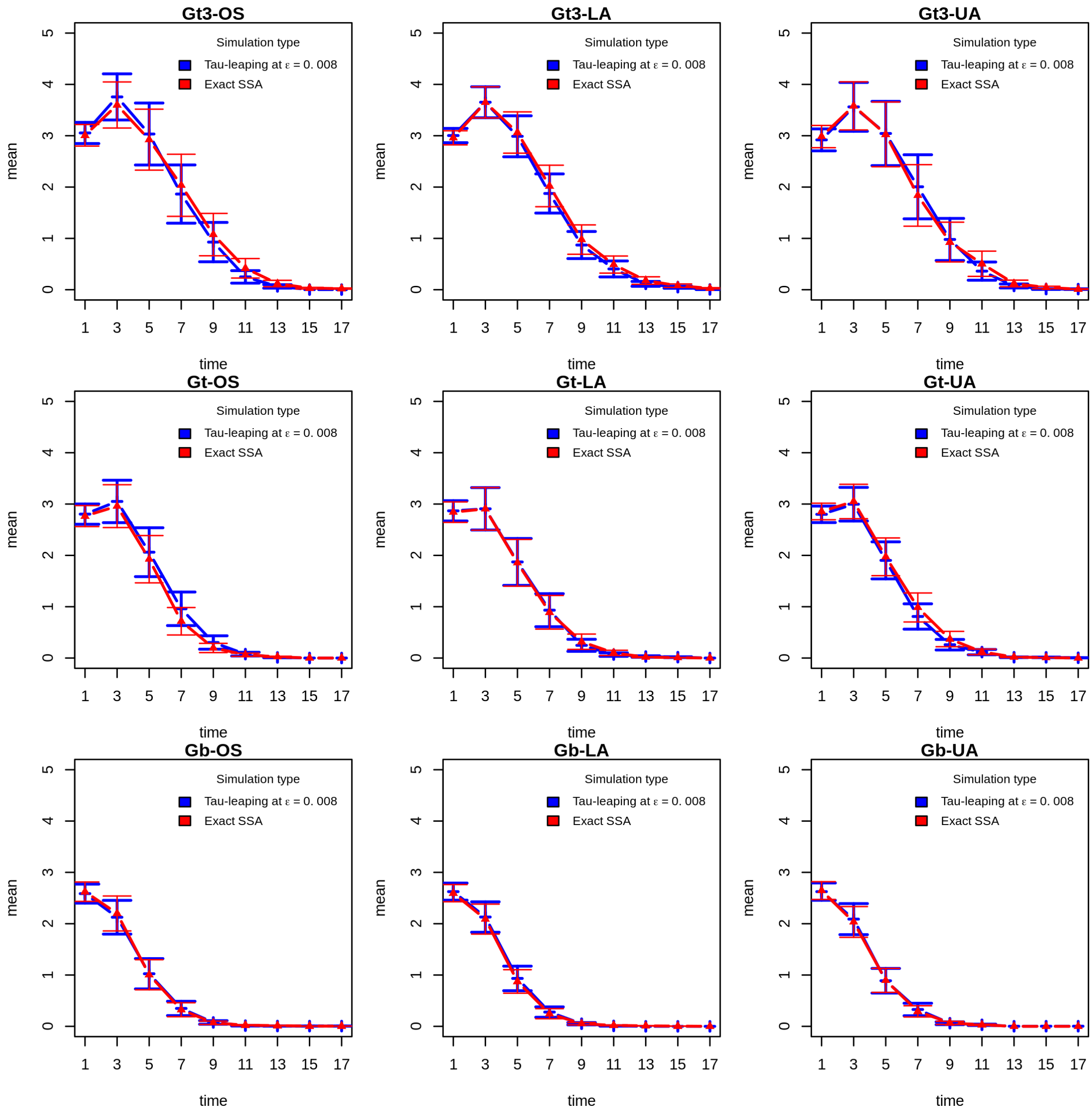

Figure 5: Mean comparison between exact SSA and Hybrid τ-leaping simulations at $\epsilon = 0.008$.

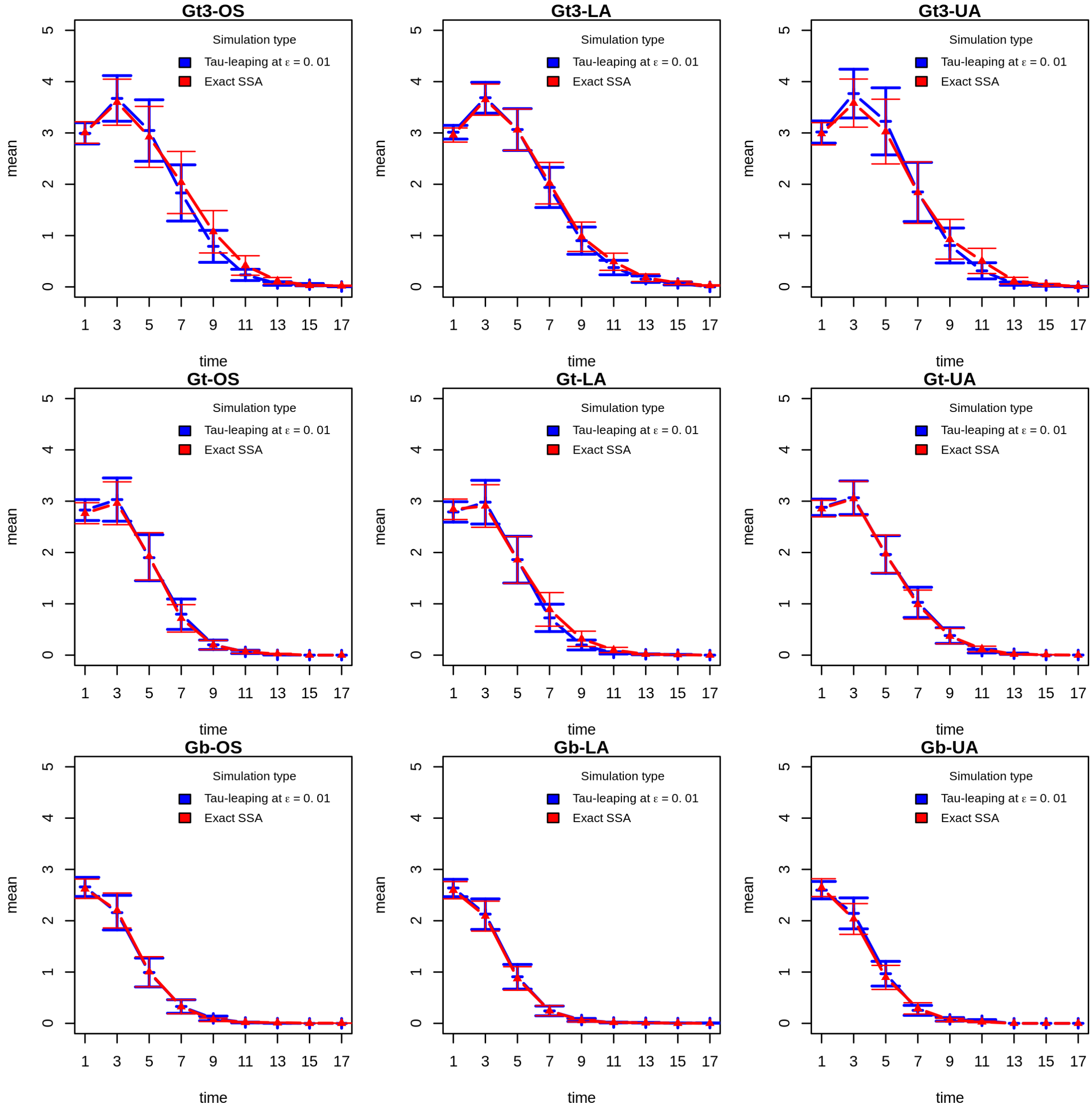

Figure 6: Mean comparison between exact SSA and Hybrid τ-leaping simulations at $\epsilon = 0.01$.

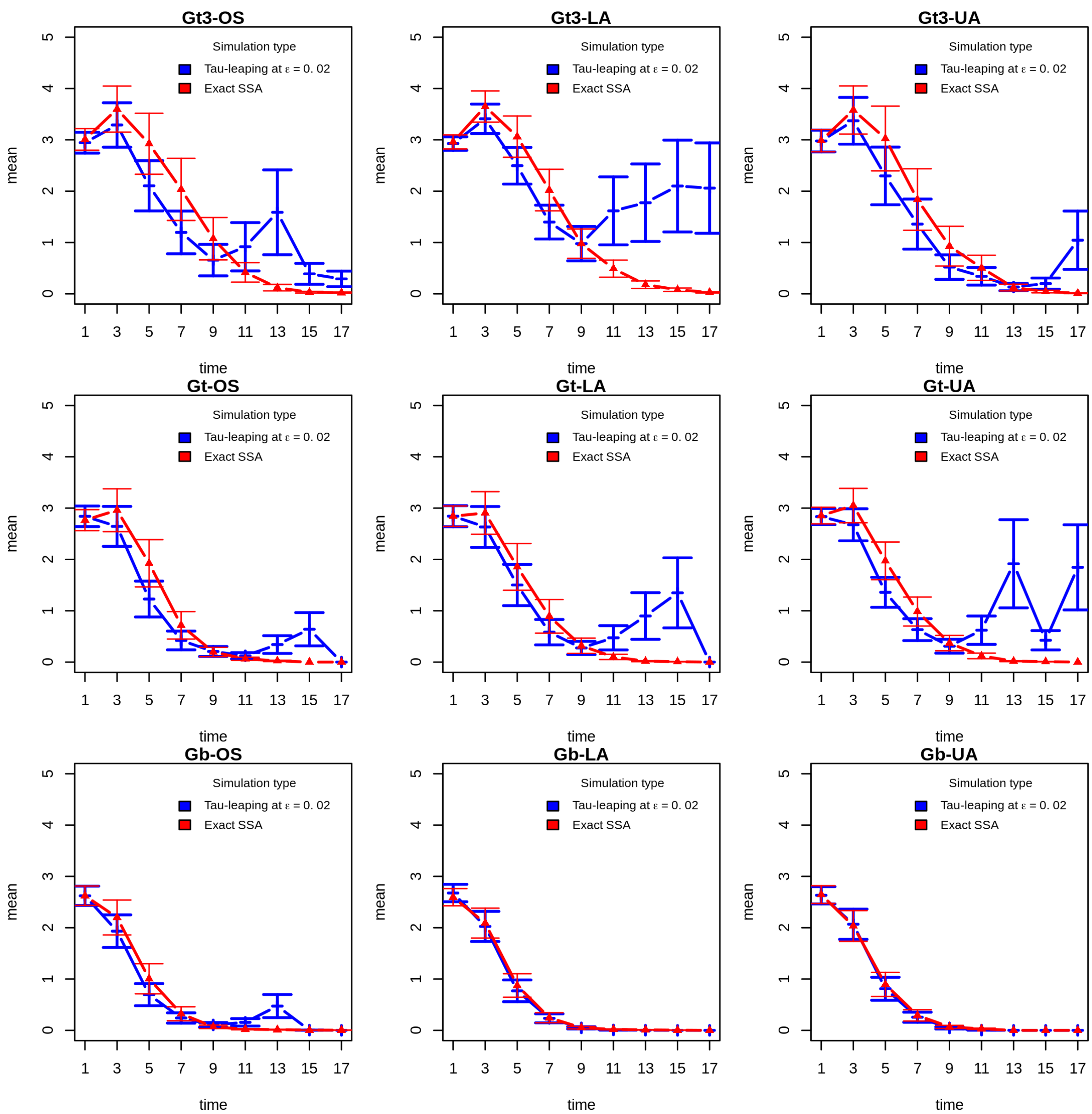

Figure 7: Mean comparison between exact SSA and Hybrid τ-leaping simulations at $\epsilon = 0.02$.

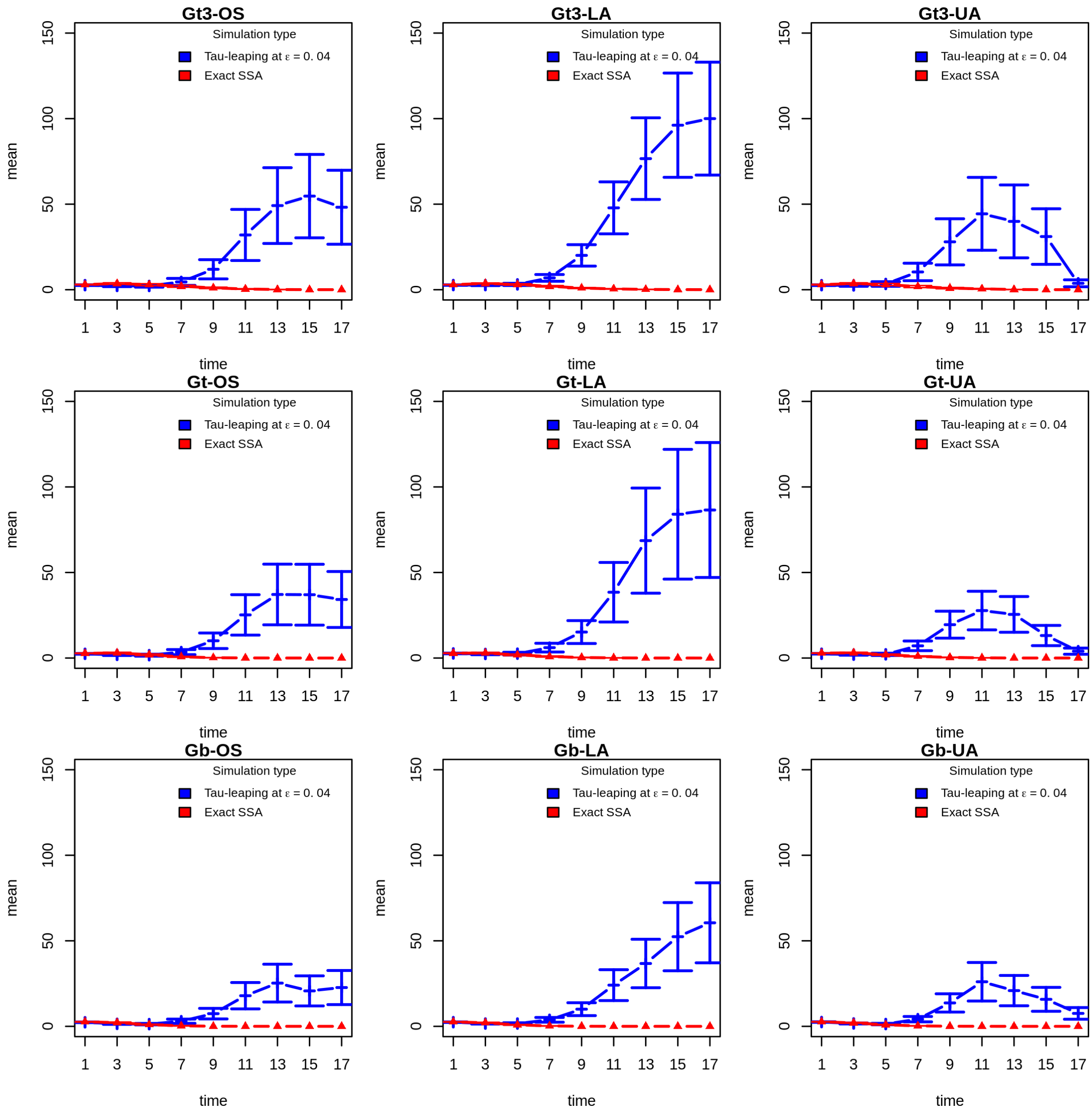

Figure 8: Mean comparison between exact SSA and Hybrid τ-leaping simulations at $\epsilon = 0.04$.

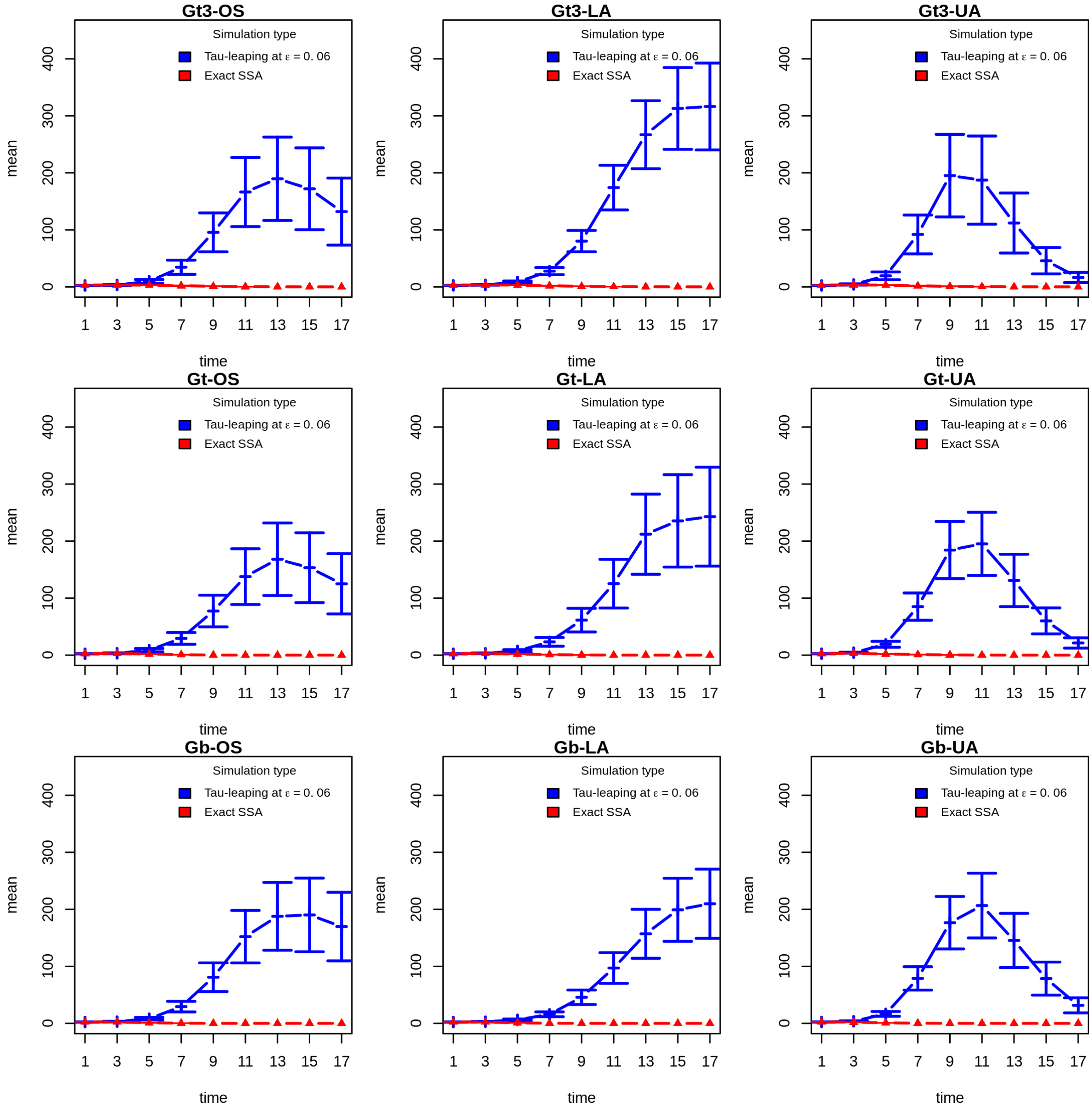

Figure 9: Mean comparison between exact SSA and Hybrid τ-leaping simulations at $\epsilon = 0.06$.

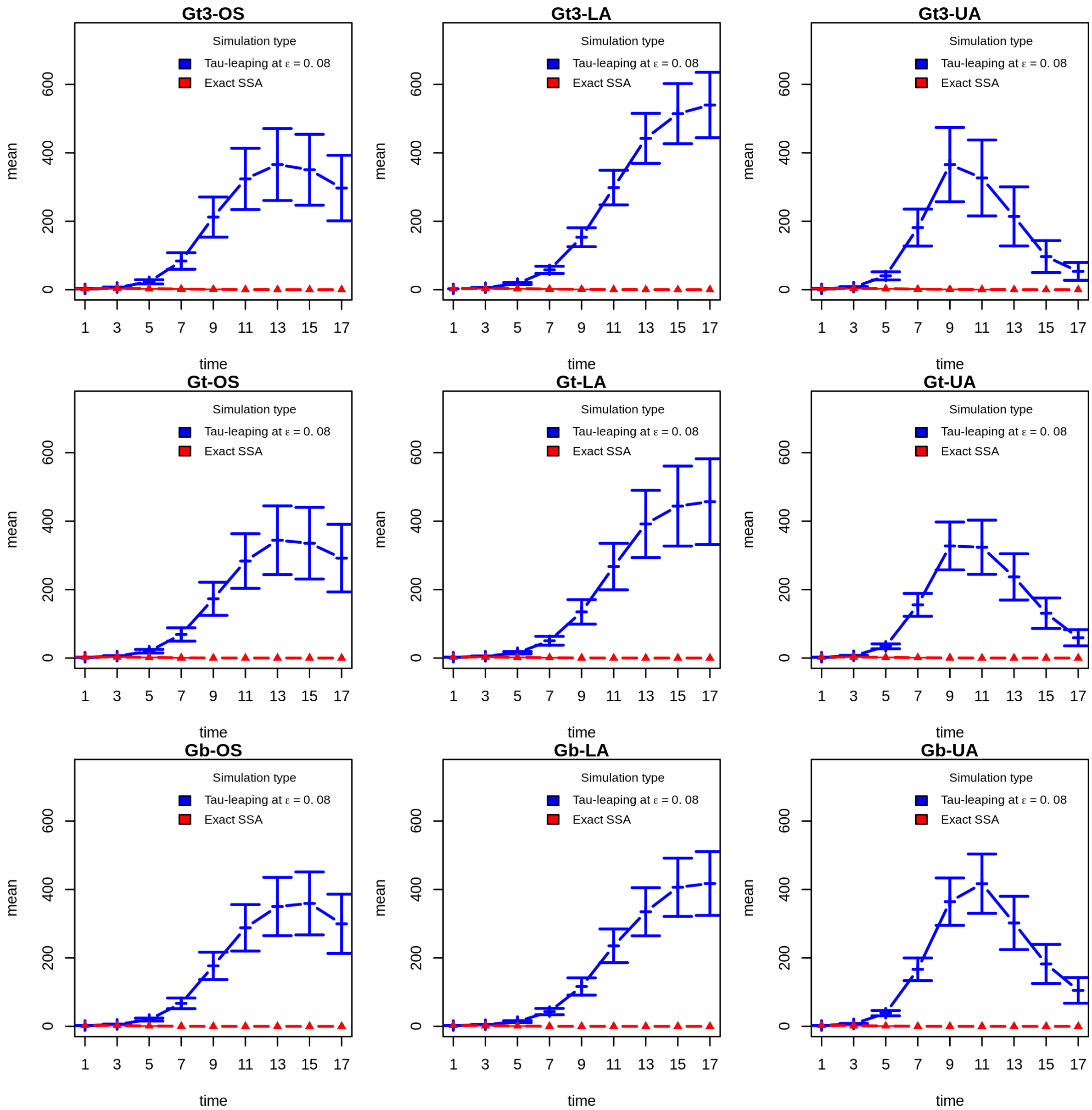

Figure 10: Mean comparison between exact SSA and Hybrid τ-leaping simulations at $\epsilon = 0.08$.

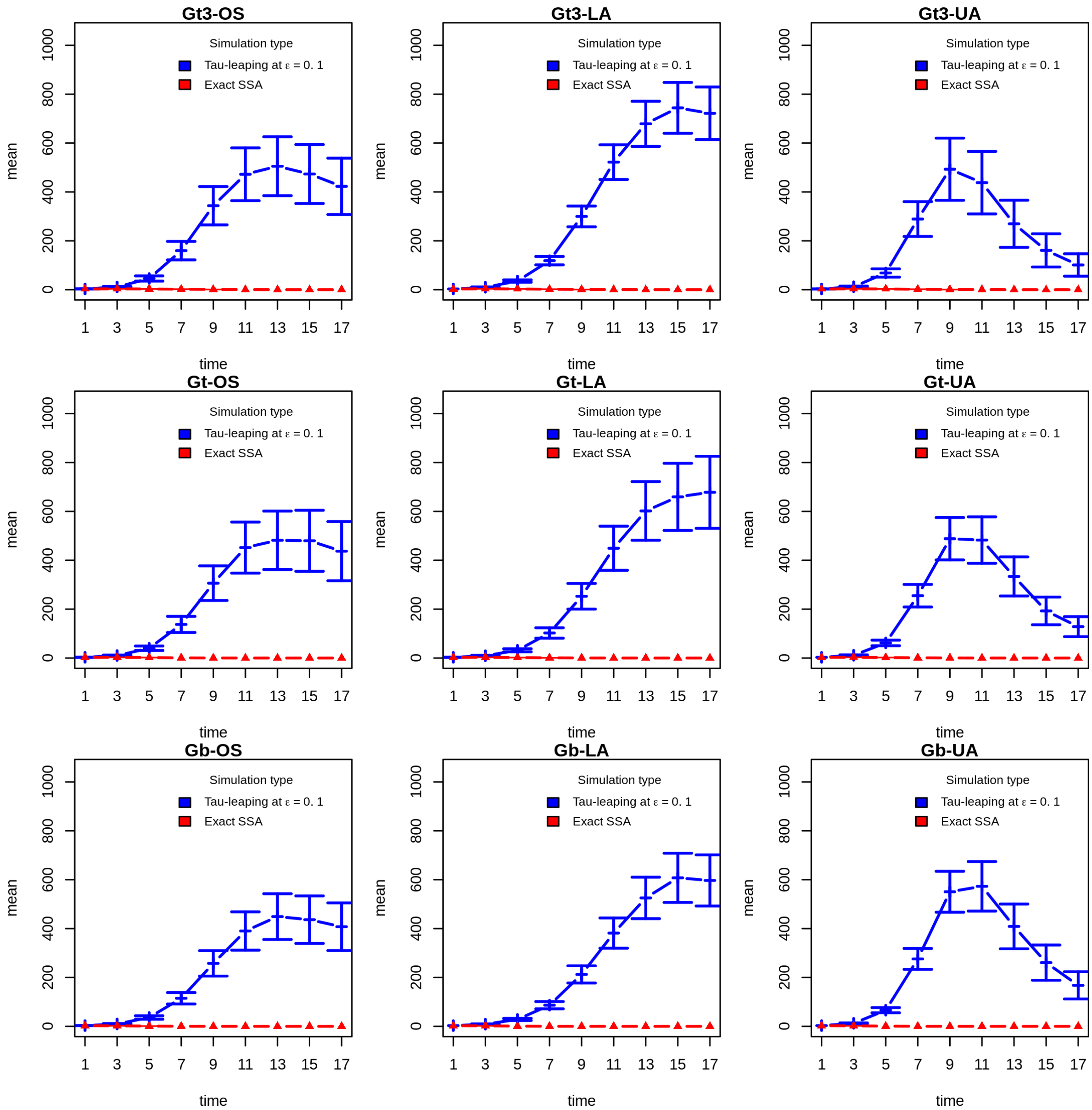

Figure 11: Mean comparison between exact SSA and Hybrid τ-leaping simulations at $\epsilon = 0.1$.

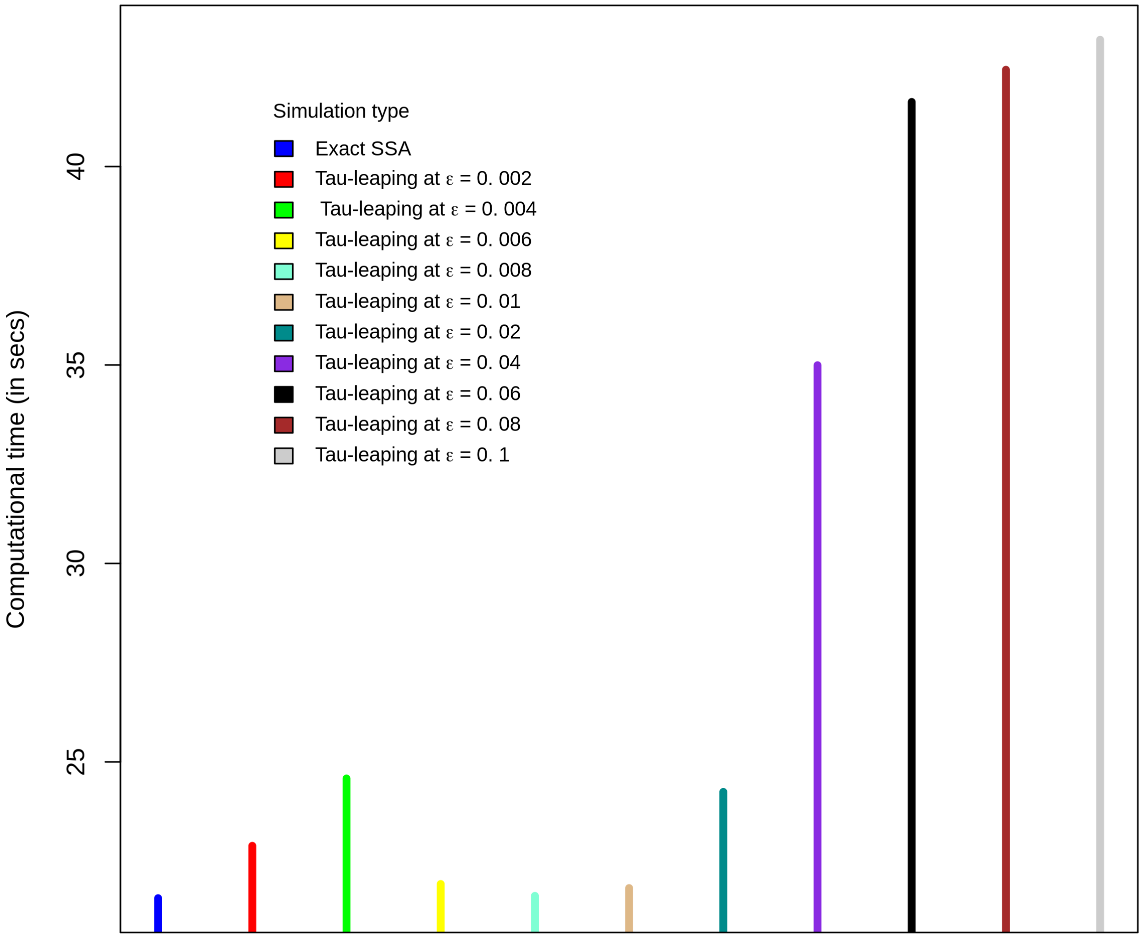

Figure 12: Comparison between computational time between exact SSA and Hybrid τ-leaping simulation at different error bounds $0 < \epsilon \leq 0.1$.