Algorithm 1 TSM-ROM-Based Transitional MCMC for 5-Species Biofilm Model

Inputs:
  Experimental data y at observation times $\{t_i\}_{i=1}^{N_t}$ for 5 species
  Prior distribution $p(\theta)$ on 20-dimensional parameter vector θ
  Observation noise variance σ_{obs}^2
  TSM-ROM likelihood evaluator $\mathcal{L}_{\text{TSM}}(\theta) = \log p(y \mid \theta)$
  Number of particles N, number of stages S, number of chains C
  Target ESS ratio ρ_{ESS}, mutation settings (proposal covariance, steps per stage)

Initialization:
for $c = 1, \ldots, C$ **do**
  for $i = 1, \ldots, N$ **do**
    Draw initial particle $\theta_i^{(0,c)} \sim p(\theta)$
    Compute log-likelihood $\ell_i^{(0,c)} \leftarrow \mathcal{L}_{\text{TSM}}\Big(\theta_i^{(0,c)}\Big)$
  end for
end for
Set initial inverse temperature $\beta_0 \leftarrow 0$

For stages $s = 1, \ldots, S$**:**
Determine next inverse temperature $\beta_s > \beta_{s-1}$ by solving for

$$\text{ESS}(\beta_s) = \frac{\Big(\sum_{i,c} w_i^{(s,c)}\Big)^2}{\sum_{i,c} (w_i^{(s,c)})^2} \approx \rho_{\text{ESS}}\, CN,$$

where $w_i^{(s,c)} \propto \exp\Big((\beta_s - \beta_{s-1})\, \ell_i^{(s-1,c)}\Big)$.
for $c = 1, \ldots, C$ **do**
  (1) Re-weighting:
  for $i = 1, \ldots, N$ **do**
    Compute incremental weight

$$\tilde{w}_i^{(s,c)} \leftarrow \exp\Big((\beta_s - \beta_{s-1})\, \ell_i^{(s-1,c)}\Big)$$

  end for
  Normalize weights $w_i^{(s,c)} \leftarrow \tilde{w}_i^{(s,c)} / \sum_j \tilde{w}_j^{(s,c)}$
  (2) Resampling:
  Resample $\{\theta_i^{(s-1,c)}\}_{i=1}^N$ according to $\{w_i^{(s,c)}\}$ to obtain equally weighted particles $\{\theta_i^{(s,c)}\}_{i=1}^N$
  Set $\ell_i^{(s,c)} \leftarrow \ell_k^{(s-1,c)}$ for the corresponding resampled index k
  (3) Mutation (MCMC moves at fixed β_s**):**
  for $i = 1, \ldots, N$ **do**
    for mutation step $m = 1, \ldots, M_s$ **do**
      Propose $\theta^\star \sim q_s(\cdot \mid \theta_i^{(s,c)})$ (e.g., Gaussian random walk)
      Evaluate TSM-ROM log-likelihood

$$\ell^\star \leftarrow \mathcal{L}_{\text{TSM}}(\theta^\star)$$

      Compute Metropolis–Hastings acceptance probability

$$\alpha = \min\Big\{1, \exp\Big(\beta_s(\ell^\star - \ell_i^{(s,c)}) + \log p(\theta^\star) - \log p(\theta_i^{(s,c)})\Big)\Big\}$$

      With probability α, set $\theta_i^{(s,c)} \leftarrow \theta^\star,\ \ell_i^{(s,c)} \leftarrow \ell^\star$
    end for
  end for
  Optionally update TSM linearization point and ROM settings based on ROM error and current β_s
end for