After calibration comes posterior sampling

- Given the models, the fixed parameters and observed data we can evaluate the value of the posterior at any parameter value

$$p(\theta, \mu, \Sigma^2, \sigma^2 \mid y, \phi, E, t) \propto p(y \mid \theta, \sigma^2, \phi, E, t) p(\theta \mid \mu, \Sigma^2) p(\mu) p(\Sigma^2) p(\sigma^2)$$

- We draw a sample from it using Markov Chain Monte Carlo methods
  - We can also investigate whether or not MCMC sampler worked ok (“converged”)
  - Given a set of samples from a posterior, we can calculate the sample mean of any function of $(\theta, \mu, \Sigma^2, \sigma^2)$
    - Including its uncertainty!

Posterior predictive samples

- For model validation we can feed posterior samples into the ODE system
- Voilá : a set of posterior predictive samples
  - Given the set of modeling assumptions and data how would the pharmacokinetics evolve in time probabilistically
  - We can compare the predicted distribution to *validation* datasets!
- In addition, we can investigate the sensitivity of the model to the evolution of PFOS in time (e.g. using area-under-curve (AUC) performance metric and increasing the value of estimated parameters by 1%)