Ready

Choose a resampling scheme

adaptive binning → MAB, Voronoi
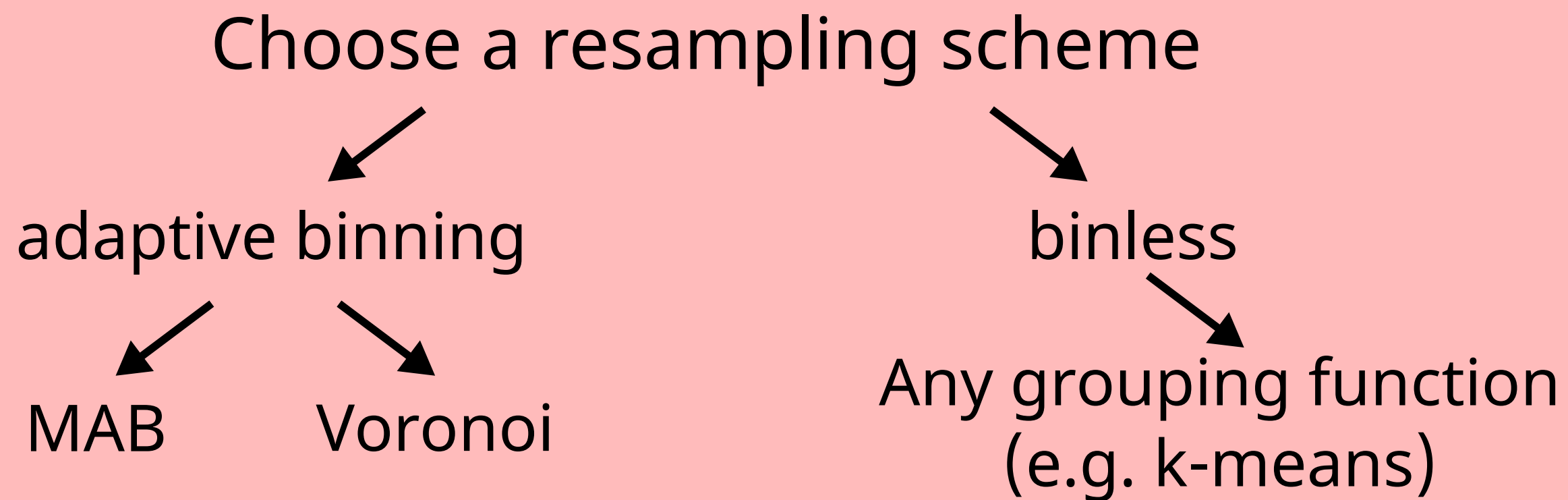
binless → Any grouping function (e.g. k-means)

Set

Generate multiple, pre-equilibrated starting conformations

Go!/Analyze

1. Run multiple, independent simulations and estimate uncertainty using the Bayesian Bootstrapping method

2. Store trajectory coordinates using the HDF5 framework

3. Assess convergence to a steady state

RED scheme   haMSM plugin   WESS plugin