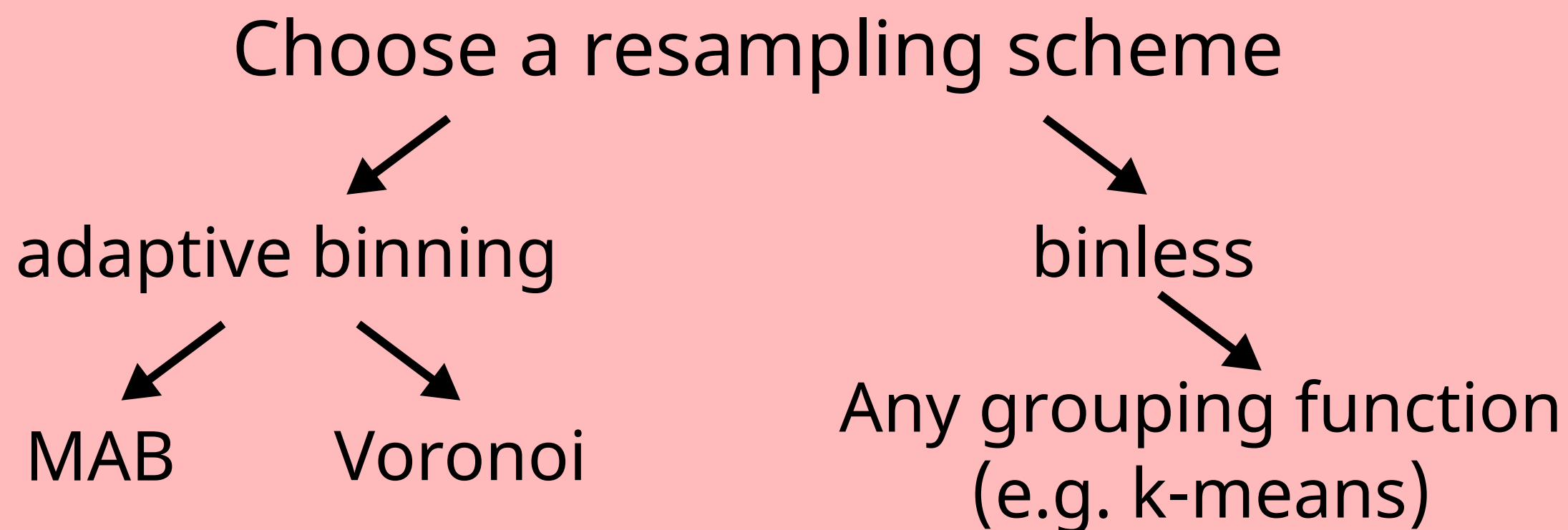


Ready

*Choose WE
simulation
parameters*



Set

*Choose system starting
configuration*

Generate multiple, pre-equilibrated
starting conformations

Go!/Analyze

*Run, monitor and analyze
the WE simulation*

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