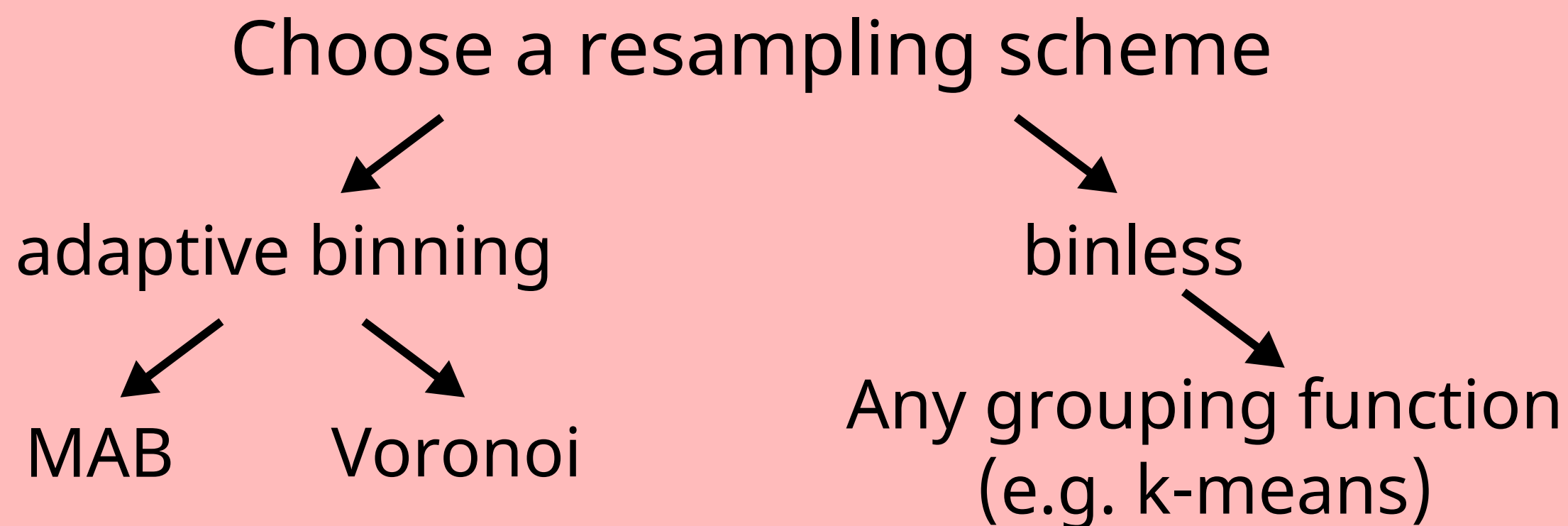


Ready

*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
-
- ```
graph TD; A[Assess convergence to a steady state] --> B[RED scheme]; A --> C[haMSM plugin]; A --> D[WESS plugin];
```
- RED scheme
- haMSM plugin
- WESS plugin