1. Shooting for replica 1 (S1)

2. Shooting for replica 2 (S2)

3. Shooting for replica 3 (S3)

4. Replica Exchange 12 (X12)















wall time

Node

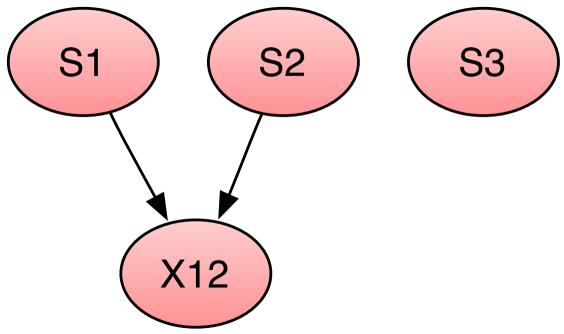
How to parallelize RETIS?

How long will trajectories be?

No idea until they run! Makes

load balancing hard....

How to avoid wasted cycles?



Moves: S1, S2, S3, X12, X23, S3, X23, S1