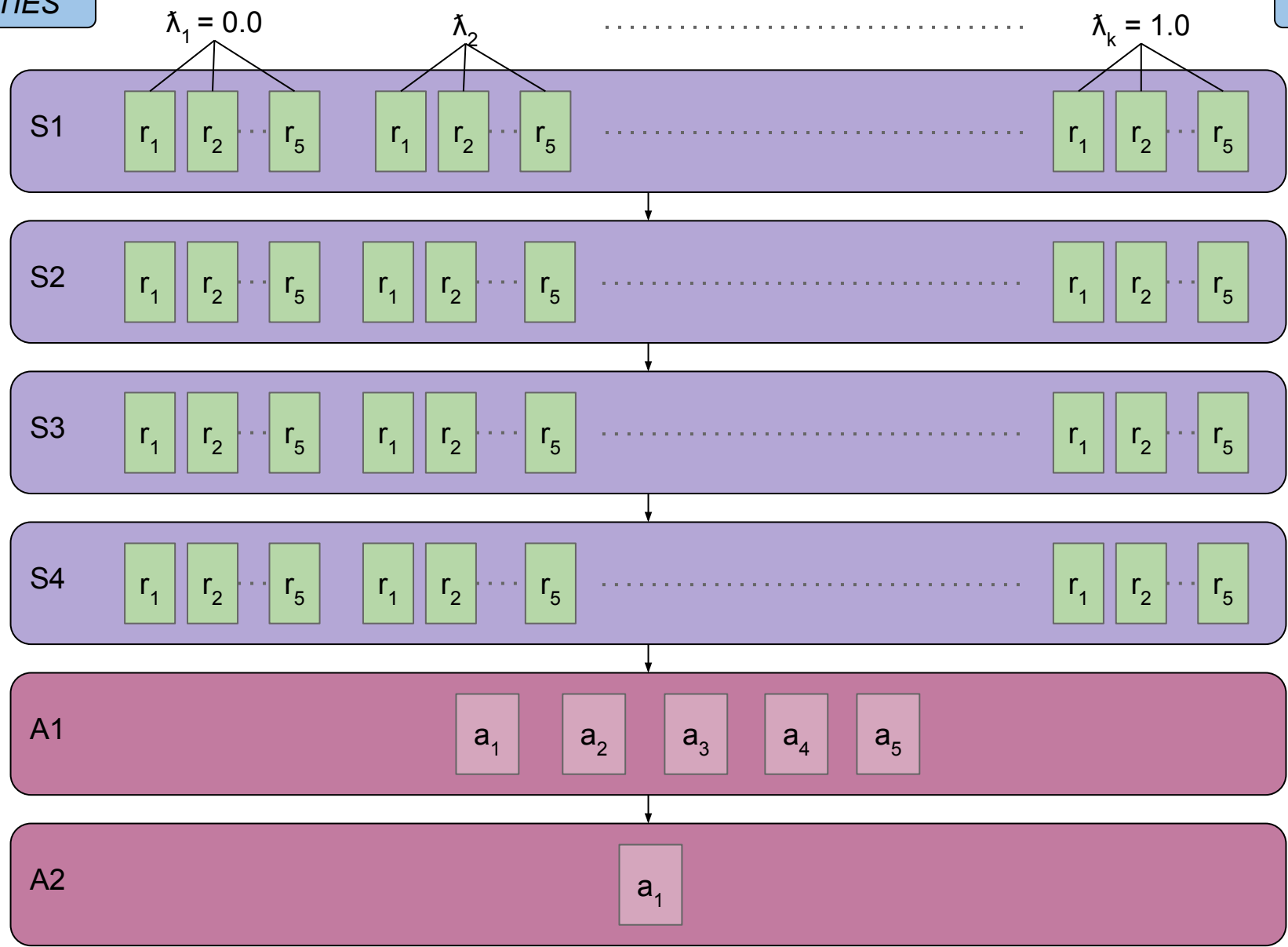
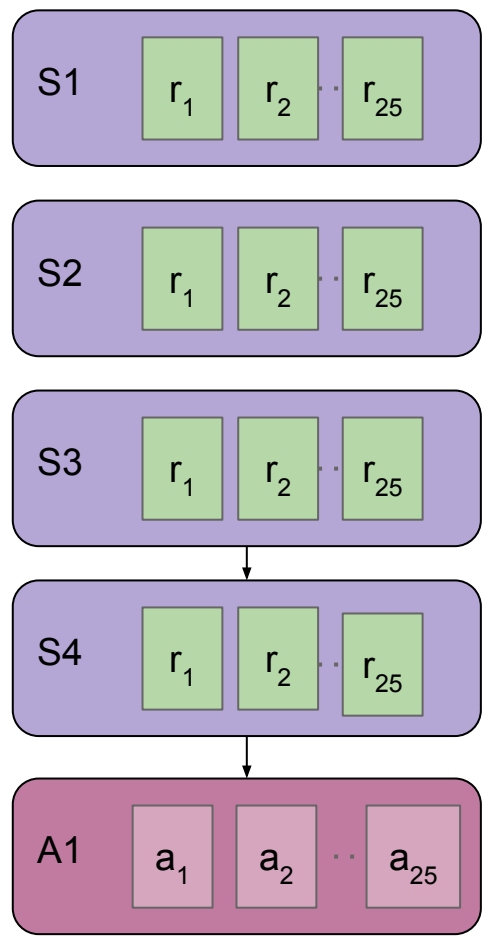


Protocol *TIES*



Protocol *ESMACS*



P Protocol

A Analysis Step

S Simulation Step

r Replica

a Analysis

S1 Minimization (NAMD)

S2 Equilibration 1 (NAMD)

S3 Equilibration 2 (NAMD)

S4 Production MD (NAMD)

A1 Local Analysis (AmberTools)

A2 Global Analysis (AmberTools)