

Main Loop

Unimolecular (branching) loop

Bimolecular (annihilation) loop

Every
timestep

Check scheduled
branching reactions

Reaction is scheduled
for this step

Choose particle at random

Choose random neighbor
site for offspring

Site occupied

Site empty

Reaction rejected

Add particle to scheduler

No reaction scheduled
for this step

All possible particles exhausted

Diffuse all particles and
do bimolecular reactions
as applicable

Iterate over all particles in
random order

At least
one left

Move to random left/right
neighbor

Site
occupied

Annihilate with probability p_A

Reaction
fails

Move is rejected; keep all
particles in current locations

Site empty

Reaction succeeds

Remove both particles
from scheduler

Has any reaction
(unimolecular or
bimolecular) occurred this
timestep?

Yes

No; continue

Reschedule next
unimolecular reaction

Choose different particle
(excluding any previous)

Move is accepted