Algorithm 1 rGFRD

while $t <$ final time **do**
  pair list $\leftarrow$ Make Pairs
  $t_{\max 1} \leftarrow$ Particle Particle Diffusion
  $t_{\max 2} \leftarrow$ Particle Boundary Diffusion
  $\Delta t_{\max} = min\ \{t_{\max 1}, t_{\max 2}\}$
  $\{\Delta t_a,\ \Delta t_r,\ \Delta t_m\} \leftarrow$Draw Event Time
  $\Delta t_s \leftarrow \min\{\Delta t_{\max},\ \Delta t_a,\ \Delta t_r,\ \Delta t_m\}$
  if $\Delta t_s == \Delta t_a$ **then**
    Update System (associating pair)
  else if $\Delta t_s == \Delta t_r$ **then**
    Update System (reversible dissociation)
  else if $\Delta t_s == \Delta t_m$ **then**
    Update System (monomolecular reaction)
  else
    Update System (no reaction)
  end if
  $t \leftarrow t + \Delta t_s$
end while

Algorithm 2 Draw Event Time

for pairs ∈ {pair list} **do**
    $\{t_a\} \leftarrow$ Draw Time (association problem)
end for
for single particles **do**
    if particle ∈ {reversible dissociation list} **then**
        if particle ∈ {pair list} **then**
            $\{t_m\} \leftarrow$ Draw Time (monomolecular reaction)
        else
            $\{t_r\} \leftarrow$ Draw Time (reversible dissociation problem)
        end if
    else
        $\{t_m\} \leftarrow$ Draw Time (monomolecular reaction)
    end if
end for
$\Delta t_a \leftarrow min\,\{t_a\}$
$\Delta t_r \leftarrow min\,\{t_r\}$
$\Delta t_m \leftarrow min\,\{t_m\}$
return $\{\Delta t_a,\ \Delta t_r,\ \Delta t_m\}$

Algorithm 3 Update System (associating pair)

association for chosen pair
for single particles **do**
    Update Particle
end for
for pairs ∈ {pair list \ updated pair} **do**
    Draw Space (association problem)
    Update Space (association problem)
end for

Algorithm 4 UPDATE PARTICLE

```
1: if particle ∈ {pair list} then
2:     do nothing
3: else if particle ∈ {REVERSIBLE DISSOCIATION LIST} then
4:     state ←FIND STATE(INTERMEDIATE)
5:     if state == bound then
6:         DRAW SPACE (GAUSSIAN)
7:         UPDATE SPACE (GAUSSIAN-DIFFUSION)
8:     else
9:         DRAW SPACE (REVERSIBLE DISSOCIATION PROBLEM)
10:        UPDATE SPACE (REVERSIBLE DISSOCIATION PROBLEM)
11:    end if
12: else
13:    DRAW SPACE (GAUSSIAN)
14:    UPDATE SPACE (GAUSSIAN-DIFFUSION)
15: end if
```

Algorithm 5 UPDATE SYSTEM (REVERSIBLE DISSOCIATION)

```
1: for chosen particle do
2:     state ← FIND STATE(EXIT)
3:     if state == separation then
4:         SEPARATION
5:     else if state == bound transformation then
6:         BOUND TRANSFORMATION
7:     else
8:         UNBOUND TRANSFORMATION
9:     end if
10: end for
11: for single particles \ updated particle do
12:     UPDATE PARTICLE
13: end for
14: for pairs ∈ {pair list} do
15:     DRAW SPACE (ASSOCIATION PROBLEM)
16:     UPDATE SPACE (ASSOCIATION PROBLEM)
17: end for
```

Algorithm 6 Update System (monomolecular reaction)

if chosen particle $\notin$ {pair list} **then**
    Draw Space (Gaussian)
    Update Space (Gaussian - transform)
end if
for single particles \ updated particle **do**
    Update Particle
end for
for pairs $\in$ {pair list} **do**
    Draw Space (association problem)
    Update Space (association problem)
    if chosen particle $\in$ pairs **then**
        Transform Chosen Particle
    end if
end for

Algorithm 7 Update System (no reaction)

for single particles **do**
    Update Particle
end for
for pairs $\in$ {pair list} **do**
    Draw Space (association problem)
    Update Space (association problem)
end for