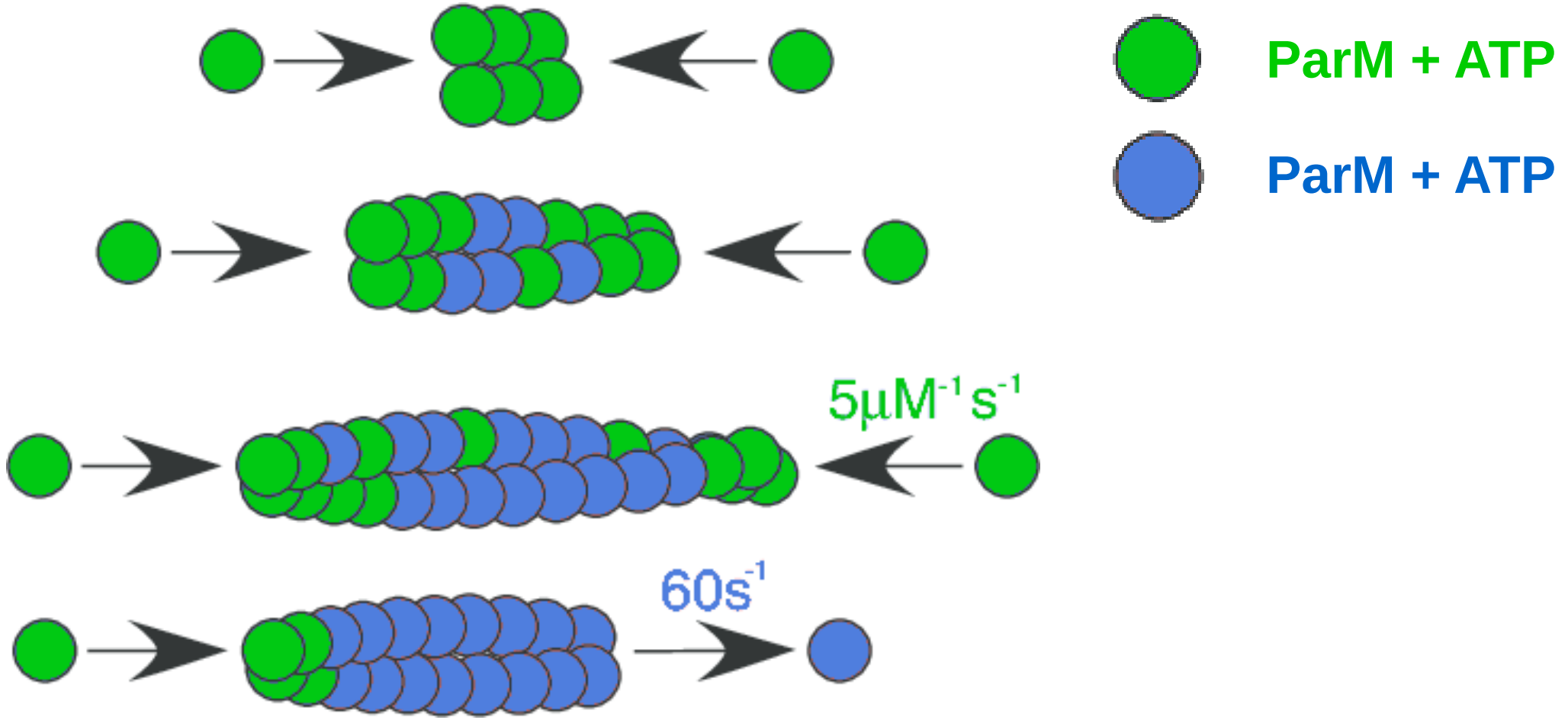
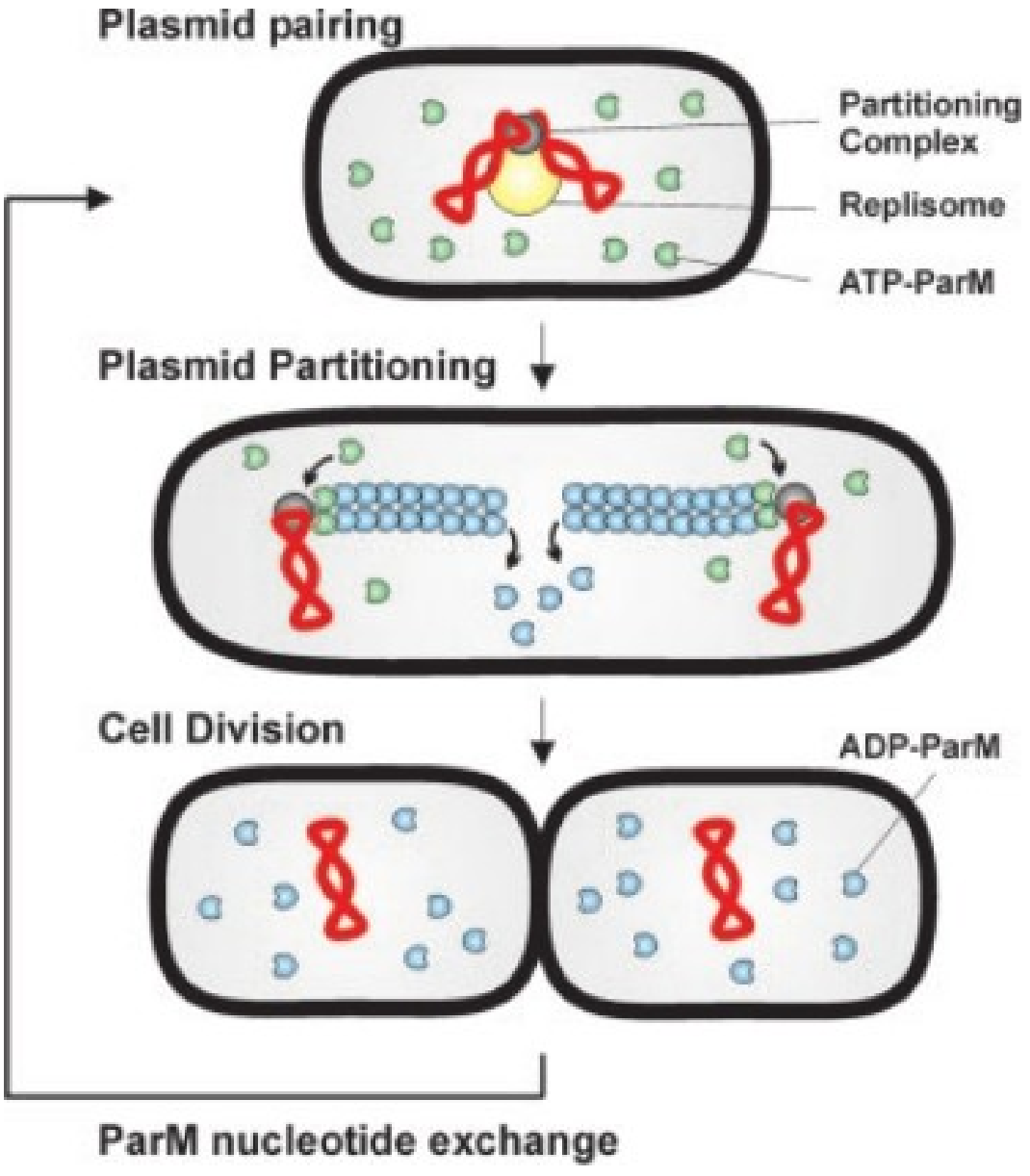
Example: Dynamic Instabilty of ParM



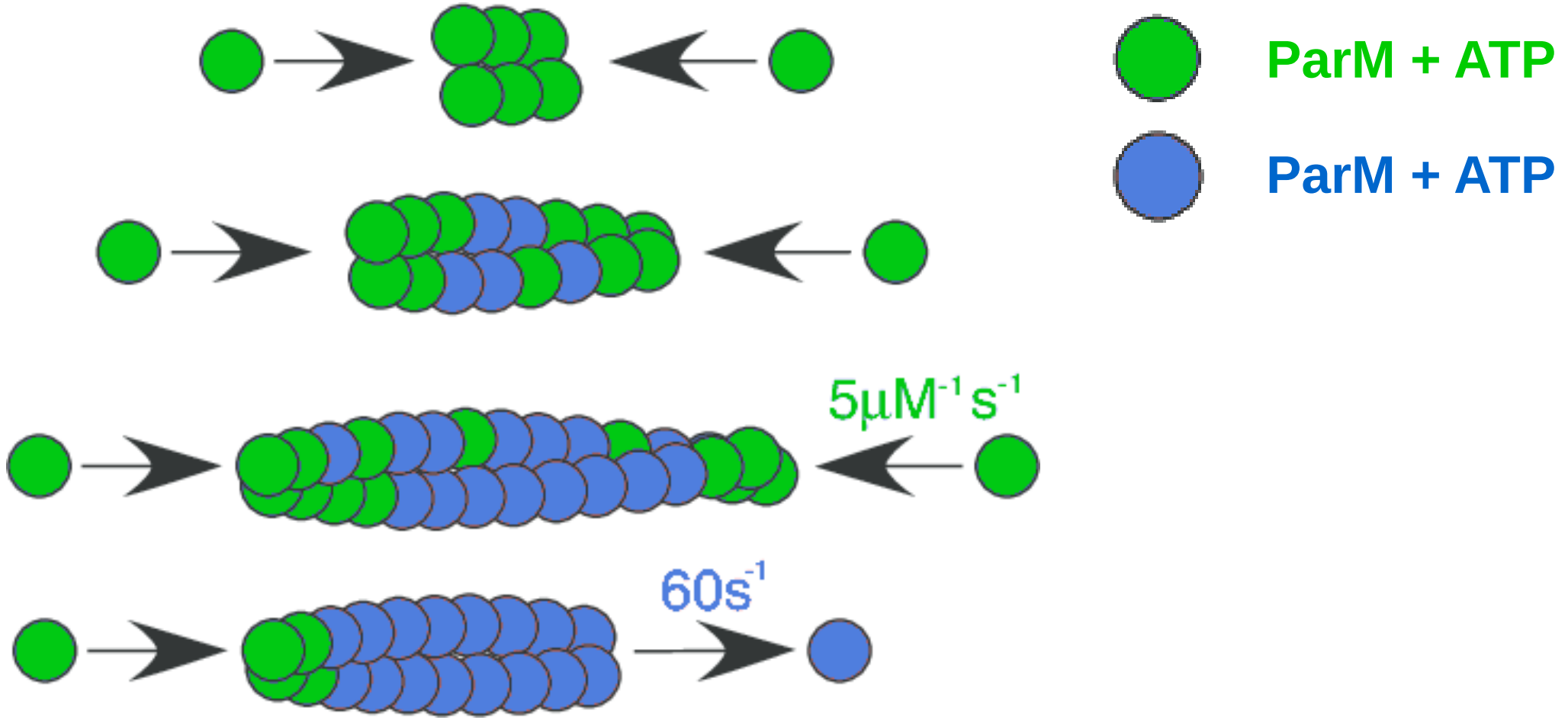
Garner, …, Mullins, Science (2004)

Example: Dynamic Instabilty of ParM



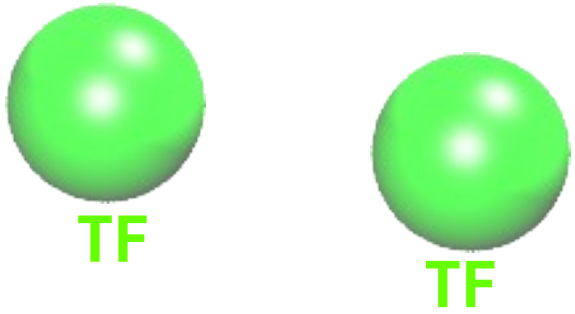
Møller-Jensen, …, Gerdes, EMBOJ (2002)

Example: Dynamic Instabilty of ParM



Garner, …, Mullins, Science (2004)

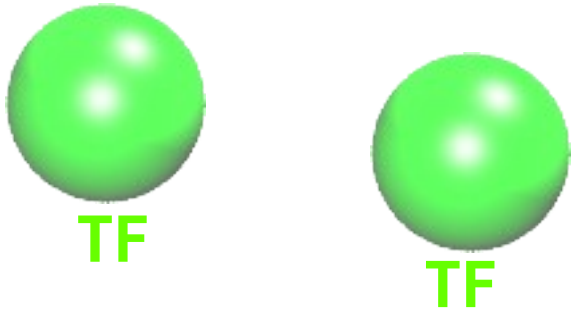
Example: Dynamic Instabilty of ParM




```
# Transition 1: Create a polymer (a dimer)

fix tr1  all  bond/new     100   delay 1                      &
  atoms @atom:TF @atom:TF and distance <= 7.1 and prob 0.1 &
-> atoms @atom:TE @atom:TE and bond @bond:F #(bond type "F")
```

Example: Dynamic Instabilty of ParM

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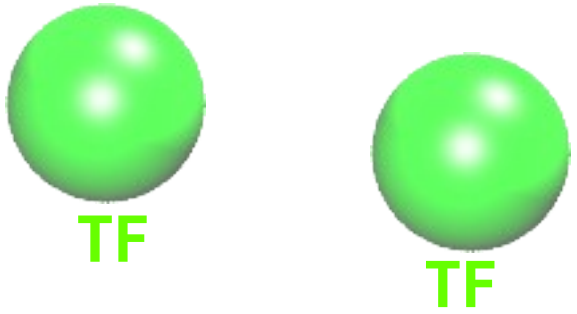
   atoms @atom:TF @atom:TF and distance <= 7.1 and prob 0.1 &
-> atoms @atom:TE @atom:TE and bond @bond:F #(bond type "F")
```

Each LAMMPS command must begin this way

(blame LAMMPS)

Example: Dynamic Instabilty of ParM

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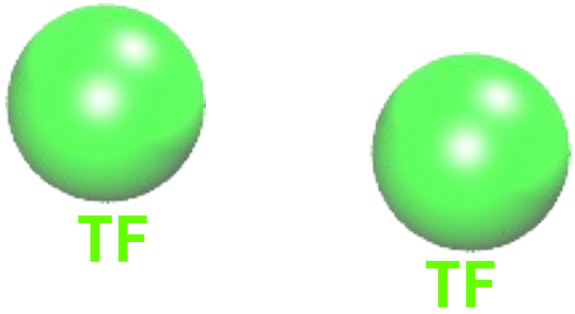
   atoms @atom:TF @atom:TF and distance <= 7.1 and prob 0.1 &
-> atoms @atom:TE @atom:TE and bond @bond:F #(bond type "F")
```

Must supply a unique name for each command (eg. "tr1")

Example: Dynamic Instabilty of ParM

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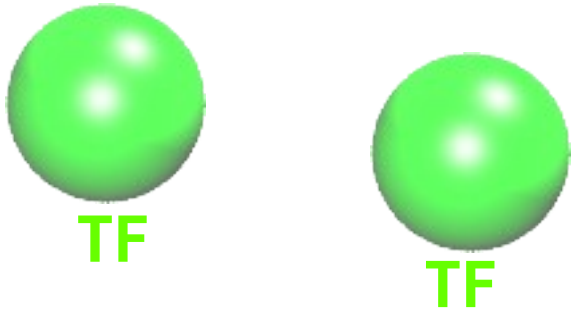
   atoms @atom:TF @atom:TF and distance <= 7.1 and prob 0.1 &
-> atoms @atom:TE @atom:TE and bond @bond:F #(bond type "F")
```

What do you want LAMMPS to do?

(eg. create a new bond bond)

Example: Dynamic Instabilty of ParM

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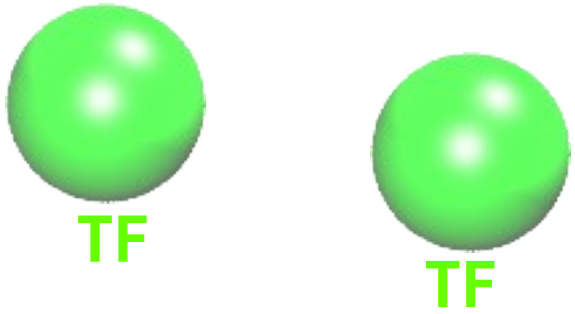
-> atoms @atom:TE @atom:TE and bond @bond:F #(bond type "F")
```

How frequently do you want LAMMPS to do it?

Example: Dynamic Instabilty of ParM

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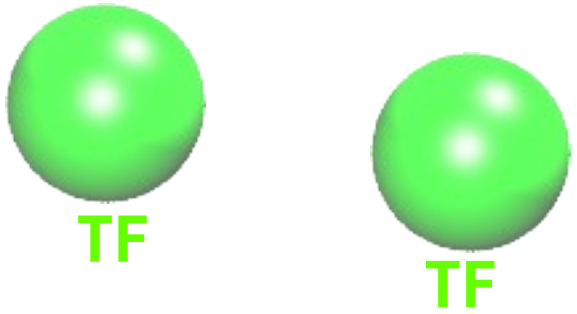
-> atoms @atom:TE @atom:TE and bond @bond:F #(bond type "F")
```

When do you want LAMMPS to do it?

(similar to a "line number")

Example: Dynamic Instabilty of ParM

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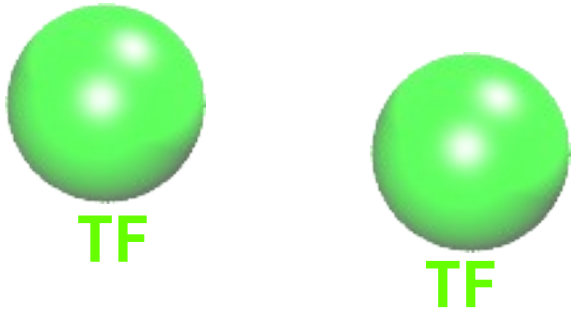


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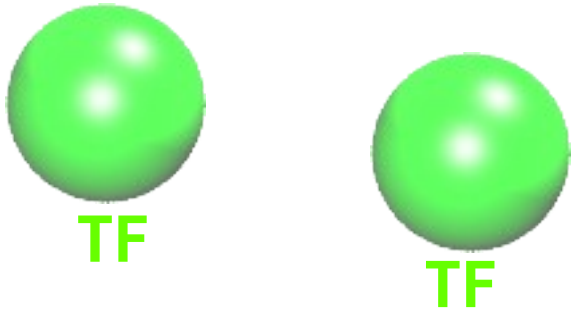


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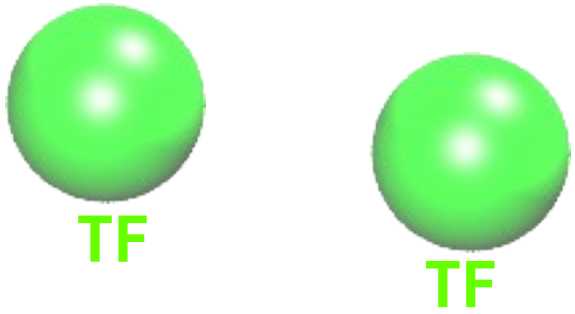
Creating a new polymer

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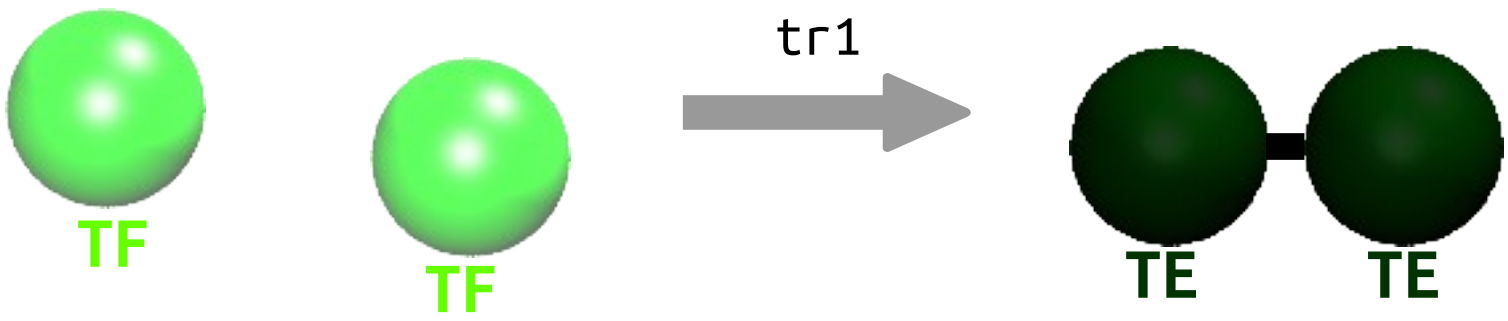
Creating a new polymer

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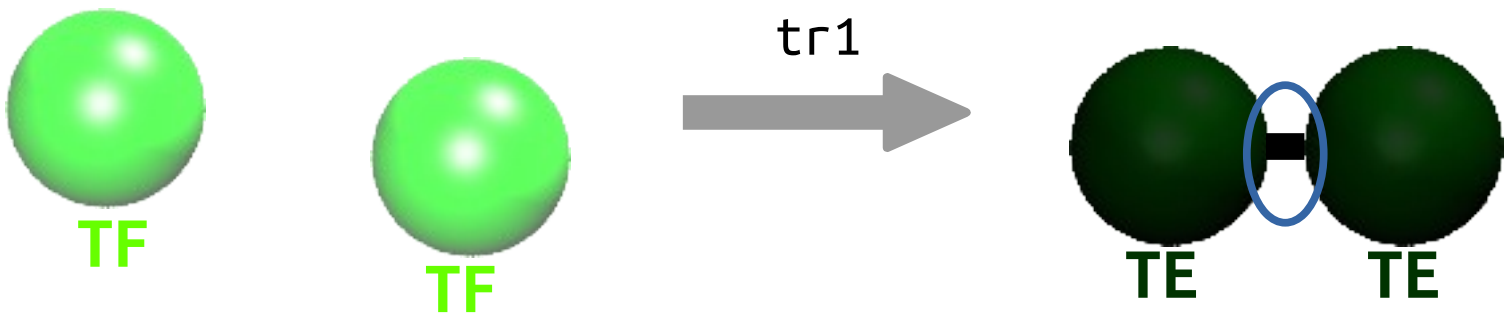


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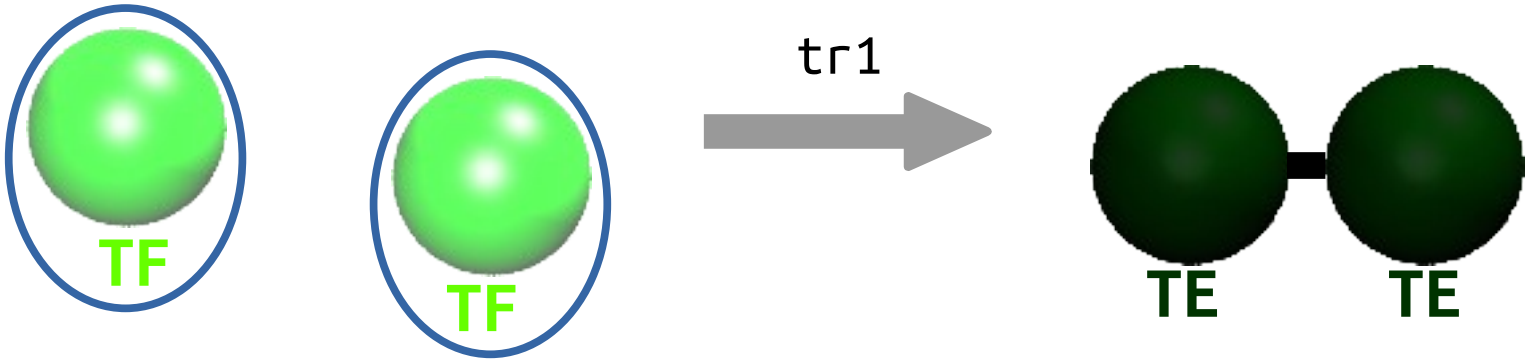


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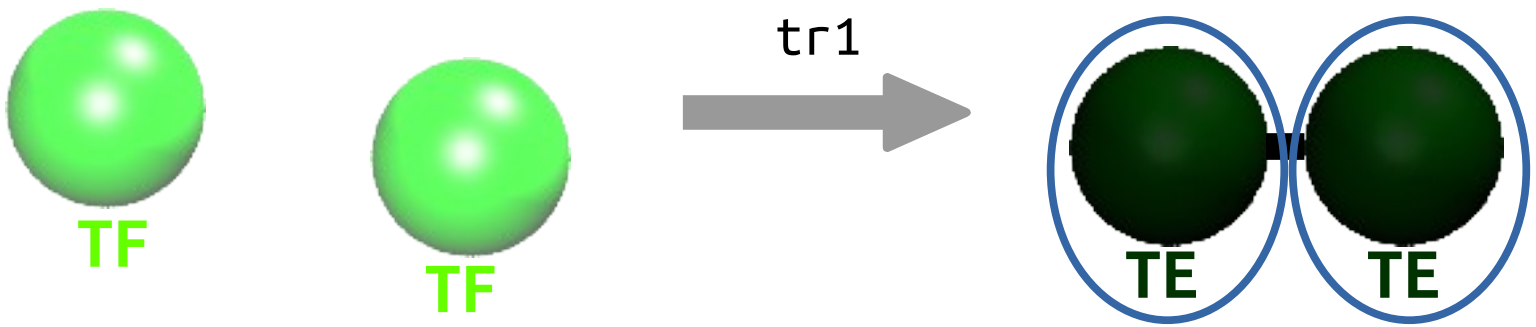
   atoms @atom:TF @atom:TF and distance <= 7.1 and prob 0.1 &
-> atoms @atom:TE @atom:TE and bond @bond:F #(bond type "F")
```

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-> atoms @atom:TE @atom:TE and bond @bond:F #(bond type "F")
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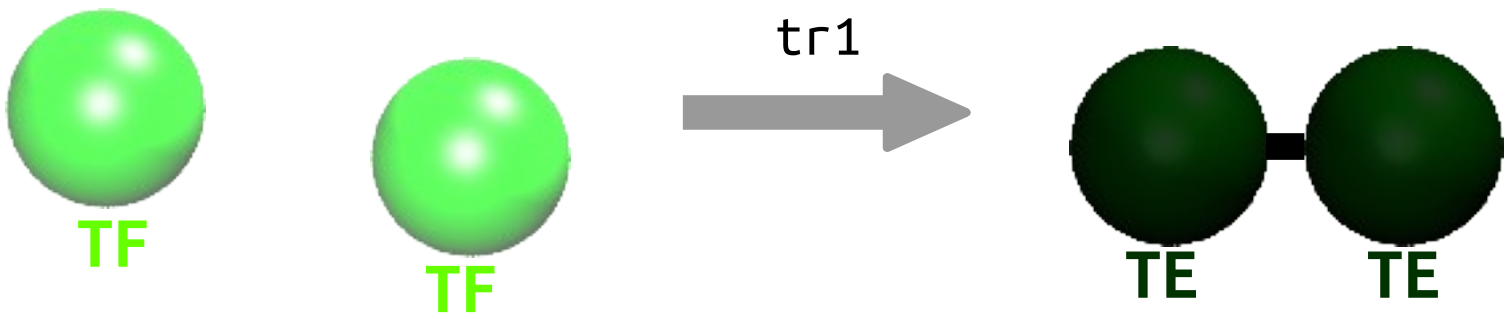
Creating a new polymer

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-> atoms @atom:TE @atom:TE and bond @bond:F #(bond type "F")
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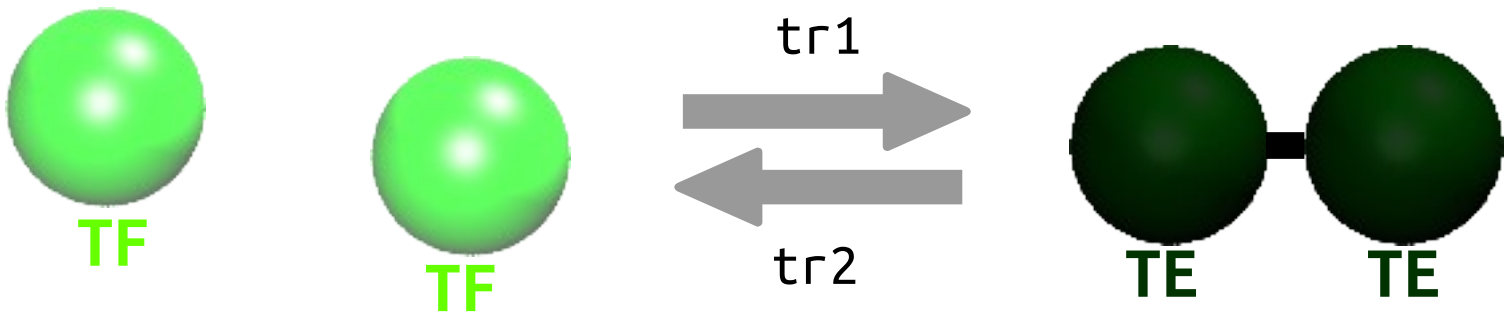
Creating a new polymer

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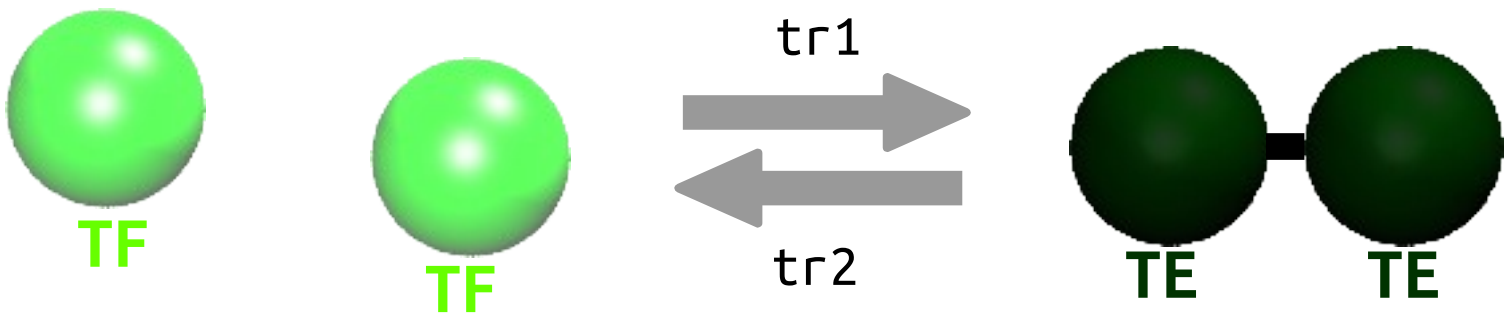
fix tr1  all  bond/new     100   delay 1                      &
  atoms @atom:TF @atom:TF and distance <= 7.1 and prob 0.1 &
-> atoms @atom:TE @atom:TE and bond @bond:F #(bond type "F")

# Transition 2: Destabilize dimers (only trimers are stable)

fix tr2  all  bond/change  100   delay 2                      &
   atoms @atom:TE  @atom:TE  and  prob 0.9                   &
-> atoms @atom:TF  @atom:TF  and  bond BREAK
```

Creating a new polymer

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-> atoms @atom:TE @atom:TE and bond @bond:F #(bond type "F")

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   atoms @atom:TE  @atom:TE  and  prob 0.9                     &
-> atoms @atom:TF  @atom:TF  and  bond BREAK
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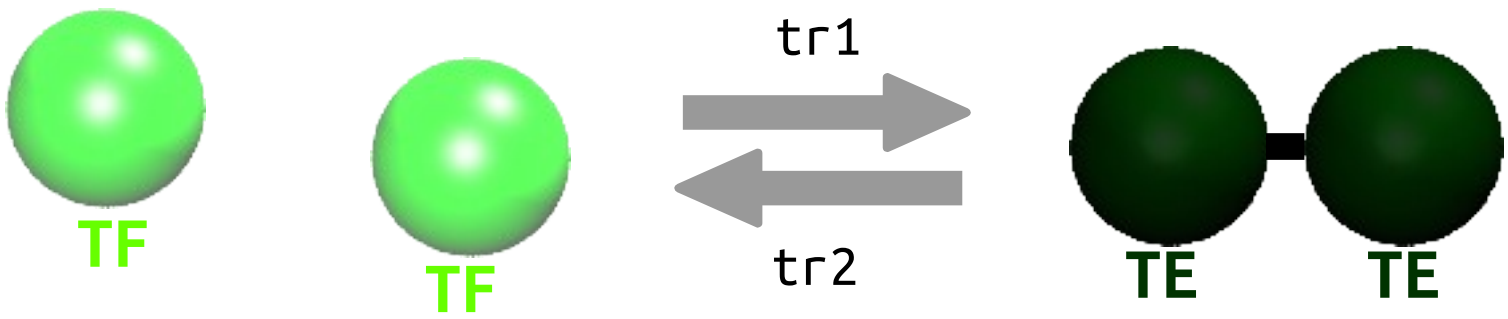


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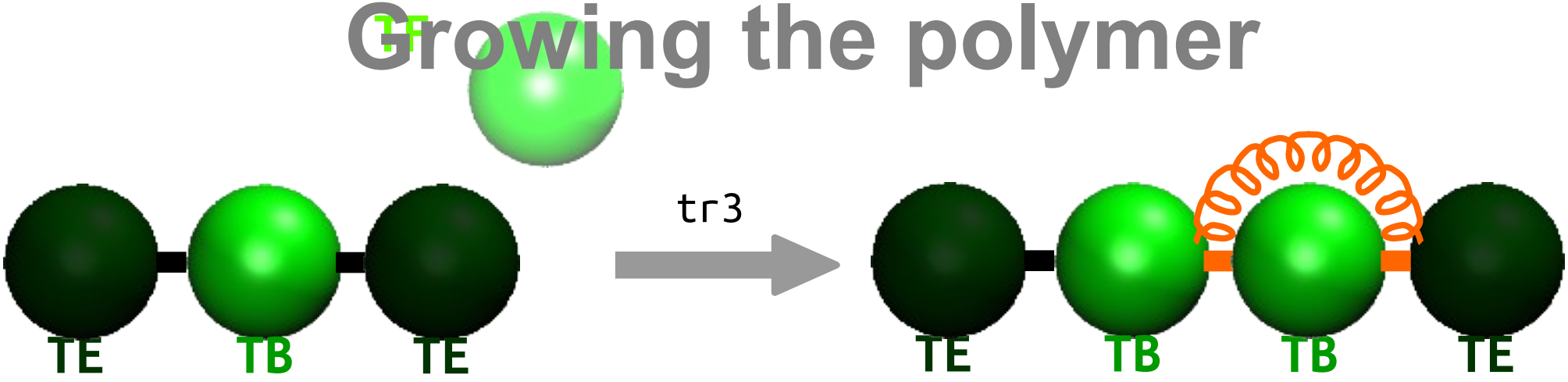
Growing the polymer

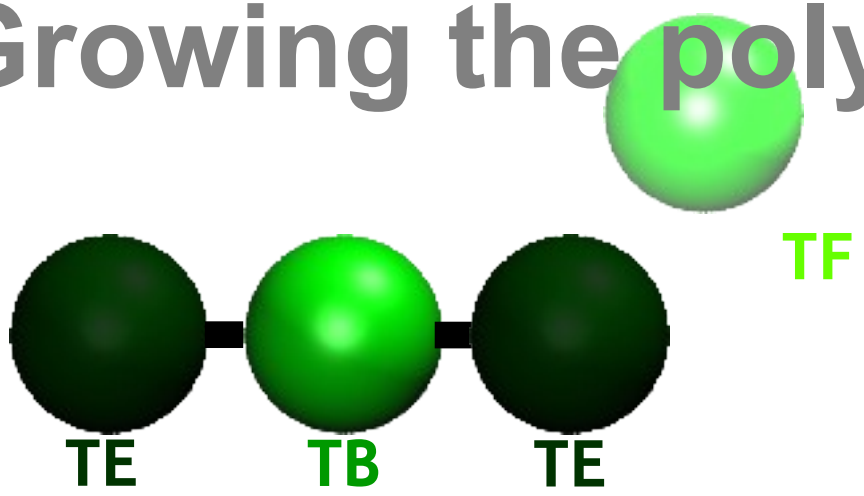



```
  # Transition 3: Attach monomers to the end of a polymer:

  fix tr3  all  bond/new     100   delay 3                      &
    atoms @atom:TE @atom:TF and distance <= 7.1 and prob 0.25 &
-> atoms @atom:TB @atom:TE and bond @bond:F  angle @angle:S TB TB TE

  angle_coeff @angle:S harmonic 851.1 180    #(persistence=10um)
```

Growing the polymer (details)

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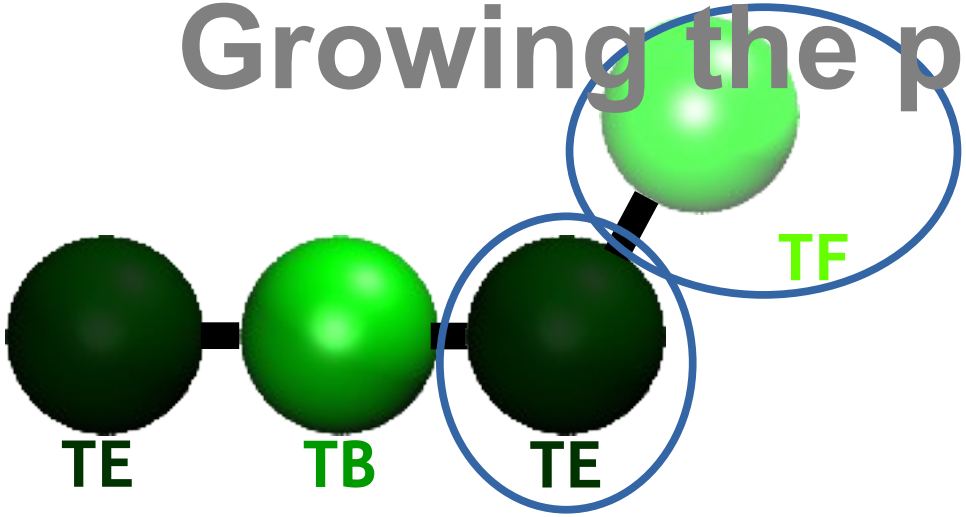
Growing the polymer

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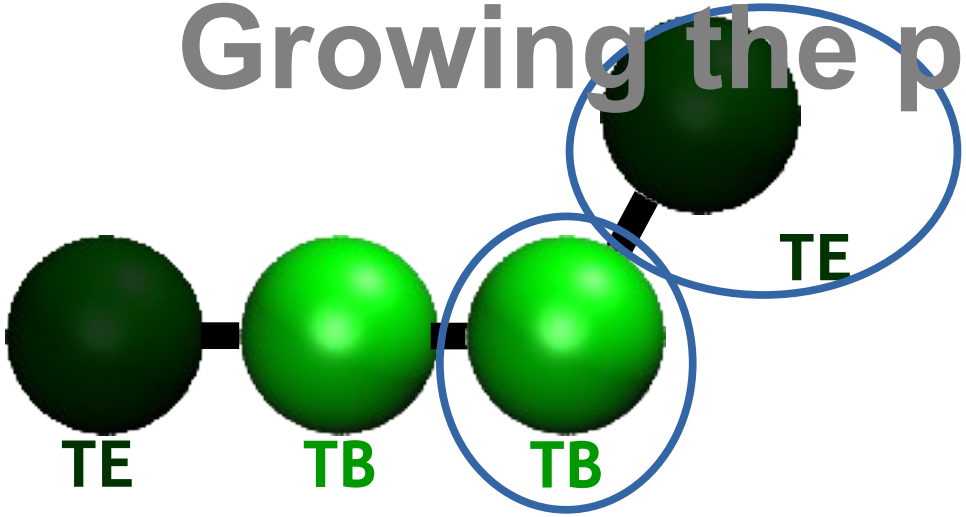
Growing the polymer

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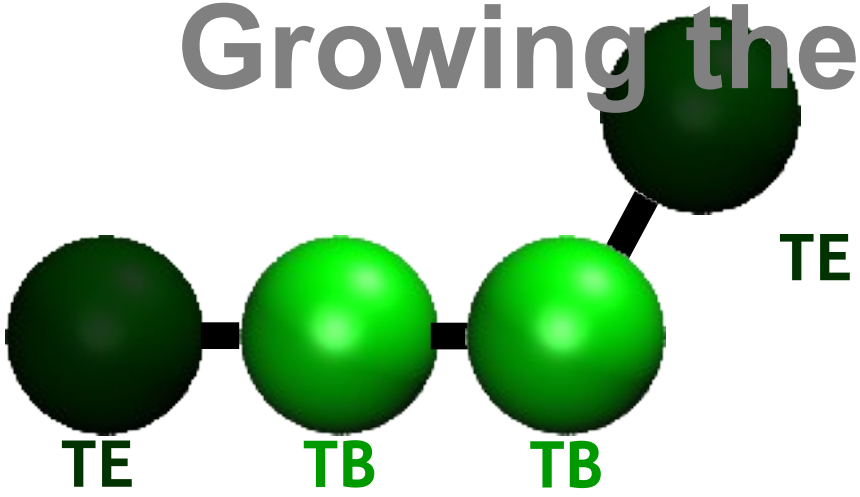
Growing the polymer

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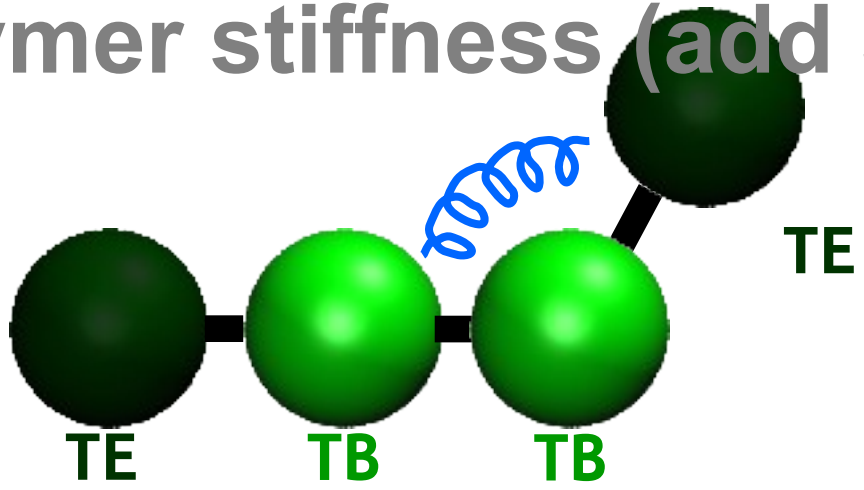
```

polymer stiffness (add 3-body interaction)



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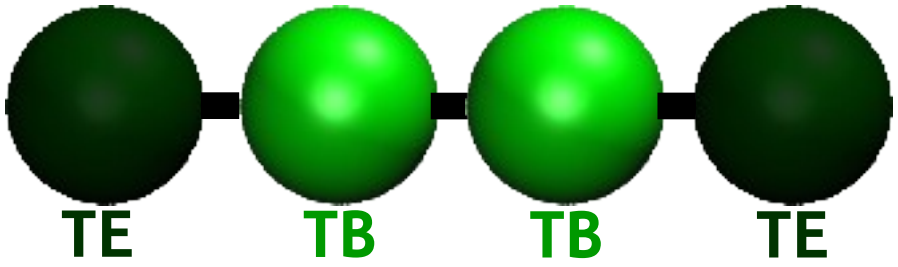


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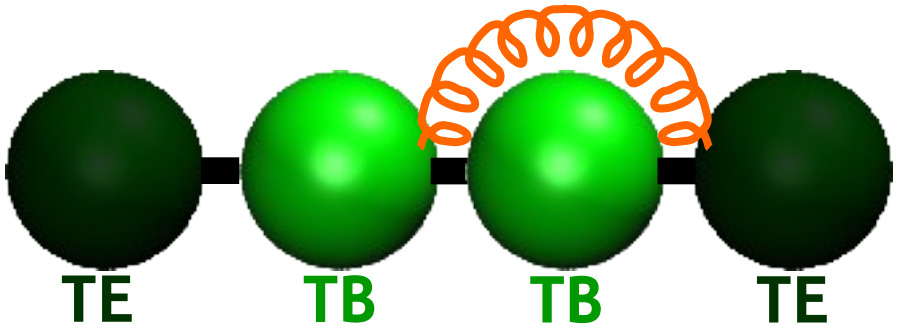


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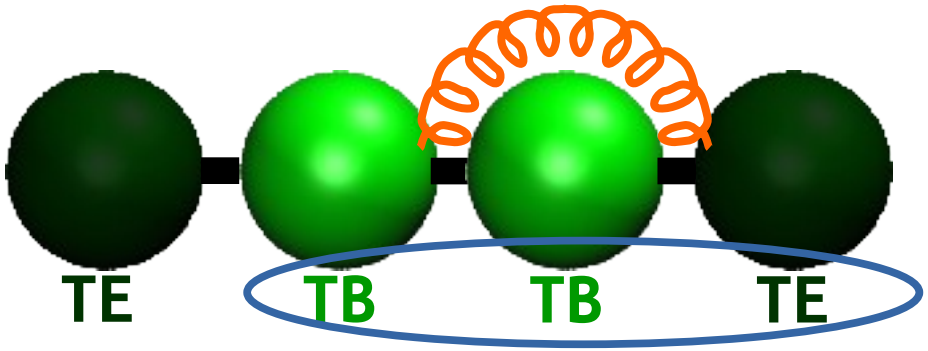


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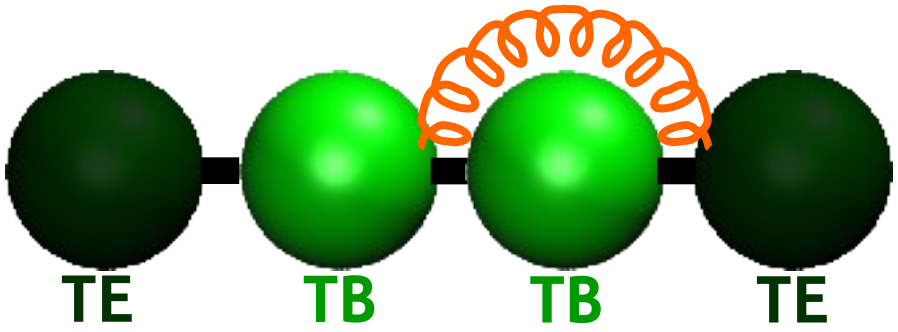


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  angle_coeff @angle:S harmonic 851.1 180    #(persistence=10um)
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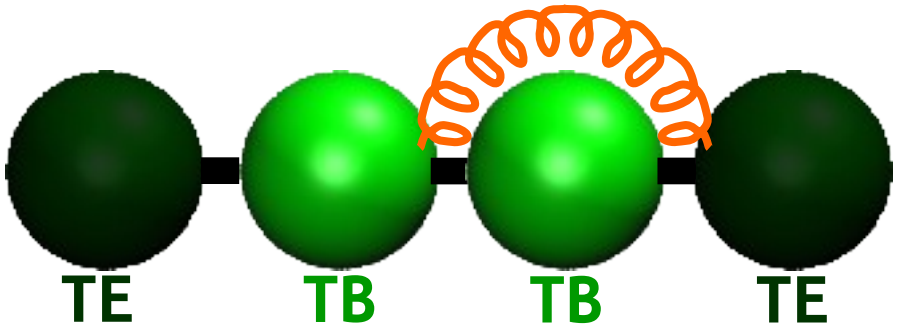
polymer stiffness (add 3-body interaction)

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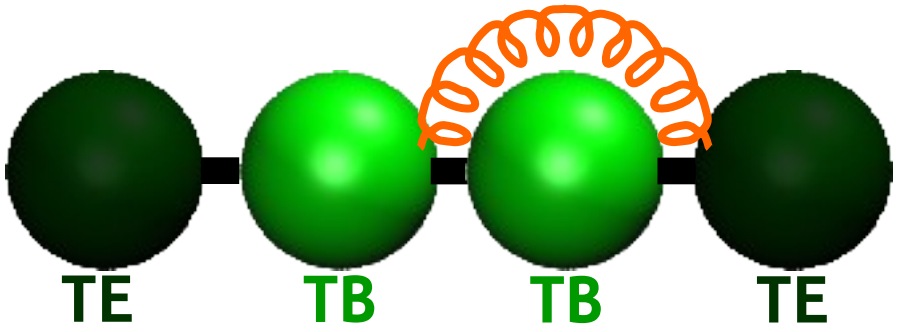


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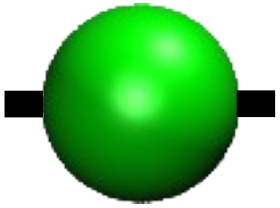
   atoms @atom:TE @atom:TF and distance <= 7.1 and prob 0.25 &
-> atoms @atom:TB @atom:TE and bond @bond:F  angle @angle:S TB TB TE

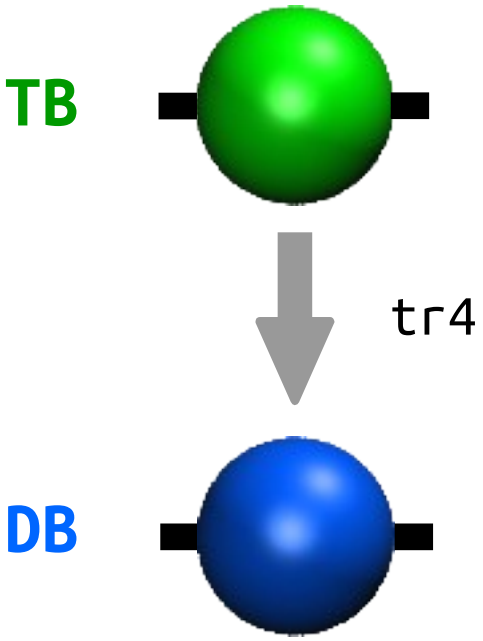
  angle_coeff @angle:S harmonic 851.1 180    #(persistence=10um)
```

maturation and depolymerization

TB 

```
# Transition 4: Hydrolize ATP  (ATP -> ADP)
fix tr4  all  atom/change  100   delay 4                    &
   atom @atom:TB and prob 0.0015 ->  ?
```

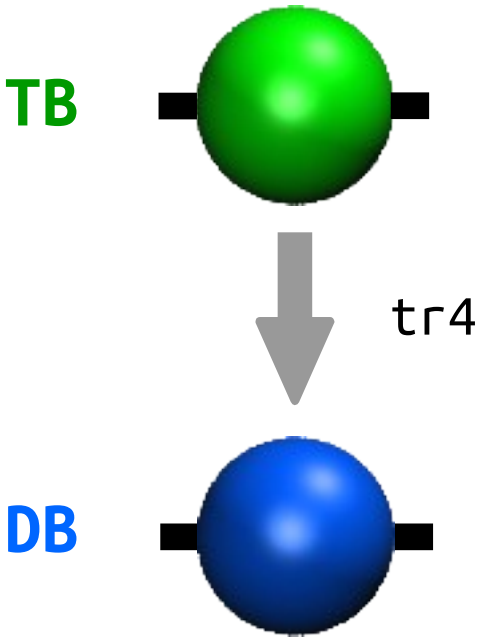
maturation and depolymerization




```
# Transition 4: Hydrolize ATP  (ATP -> ADP)

fix tr4  all  atom/change  100   delay 4                    &
   atom @atom:TB and prob 0.0015 -> atom @atom:DB
```

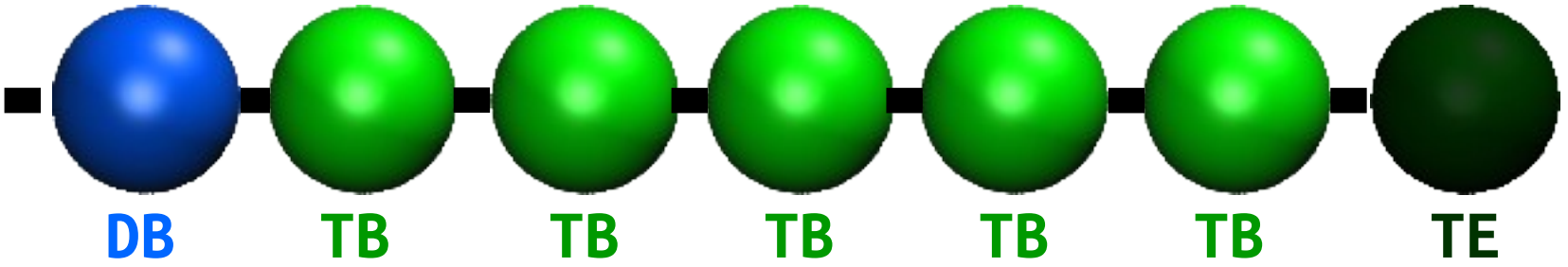
maturation and depolymerization




```
# Transition 4: Hydrolize ATP  (ATP -> ADP)

fix tr4  all  atom/change  100   delay 4                    &
   atom @atom:TB and prob 0.0015 -> atom @atom:DB
```

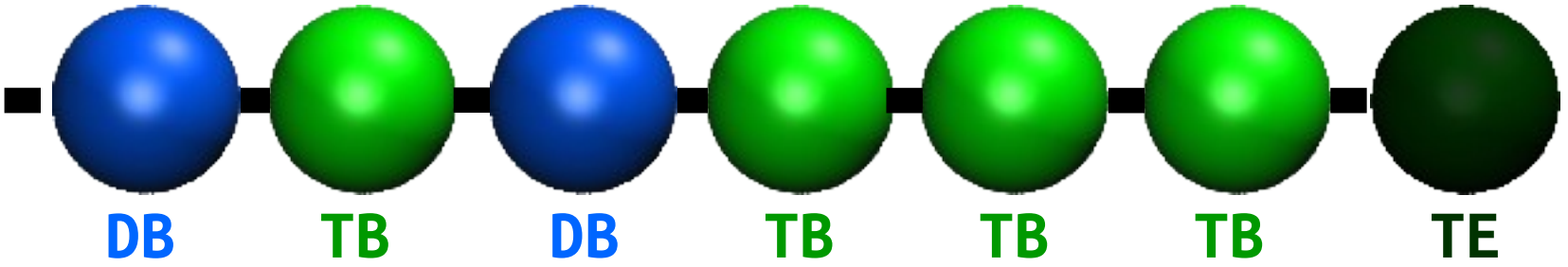
maturation and depolymerization




```
# Transition 4: Hydrolize ATP  (ATP -> ADP)

fix tr4  all  atom/change  100   delay 4                    &
   atom @atom:TB and prob 0.0015 -> atom @atom:DB
```

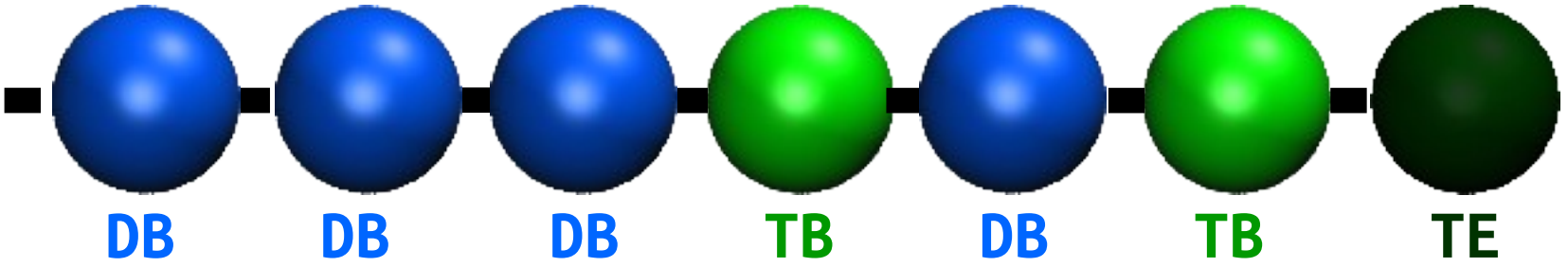
maturation and depolymerization




```
# Transition 4: Hydrolize ATP  (ATP -> ADP)

fix tr4  all  atom/change  100   delay 4                    &
   atom @atom:TB and prob 0.0015 -> atom @atom:DB
```

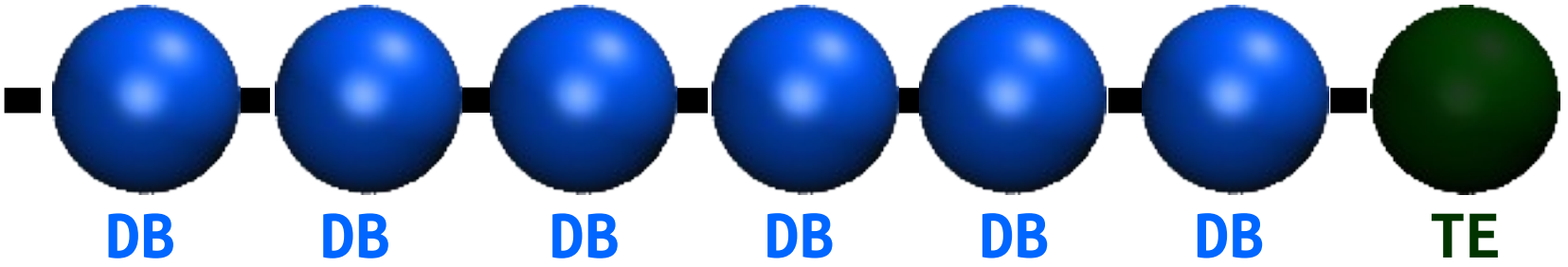
maturation and depolymerization




```
# Transition 4: Hydrolize ATP  (ATP -> ADP)

fix tr4  all  atom/change  100   delay 4                    &
   atom @atom:TB and prob 0.0015 -> atom @atom:DB
```

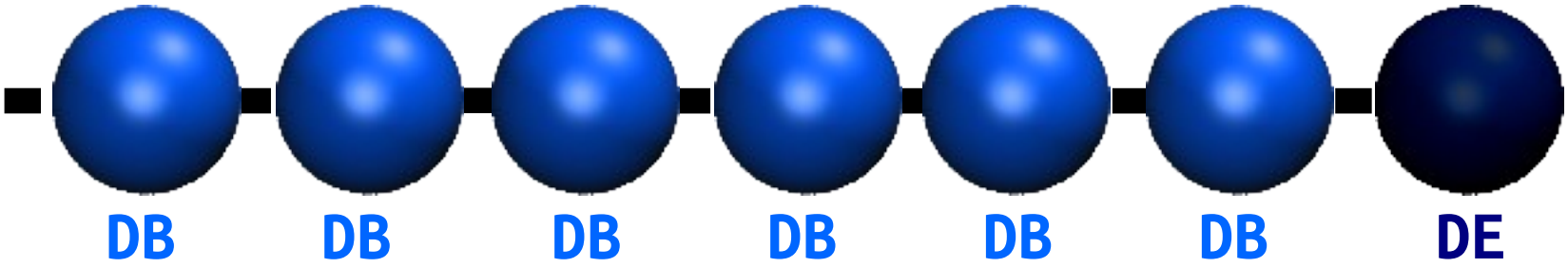
maturation and depolymerization



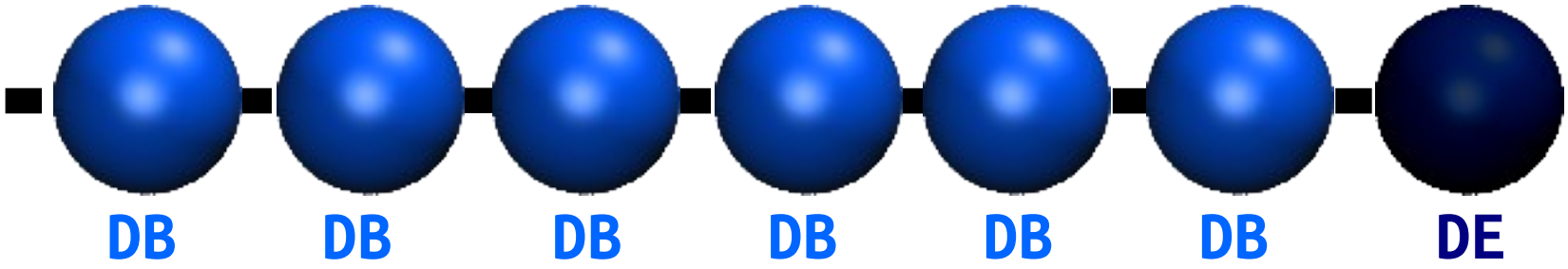

```
# Transition 4: Hydrolize ATP  (ATP -> ADP)

fix tr4  all  atom/change  100   delay 4                    &
   atom @atom:TB and prob 0.0015 -> atom @atom:DB
```

maturation and depolymerization



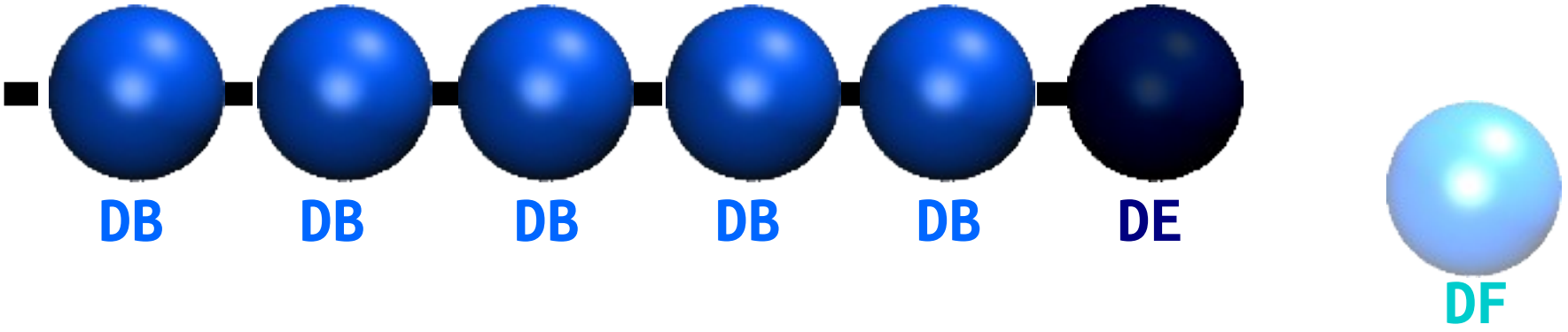
maturation and depolymerization




```
# Transitions 5: Depolymerize ADP-bound ParM at the end (DE)

fix tr6  all  bond/change  100   delay 5                    &
   atoms @atom:DB  @atom:DE                                 &
-> atoms @atom:DE  @atom:DF and bond BREAK
```

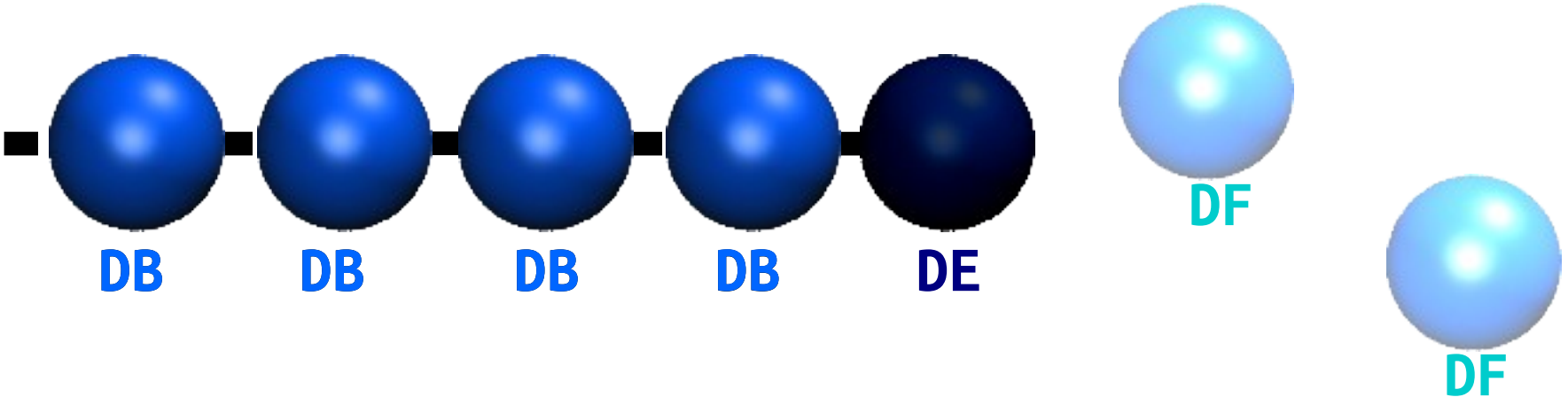
maturation and depolymerization




```
# Transitions 5: Depolymerize ADP-bound ParM at the end (DE)

fix tr6  all  bond/change  100   delay 5                    &
   atoms @atom:DB  @atom:DE                                 &
-> atoms @atom:DE  @atom:DF and bond BREAK
```

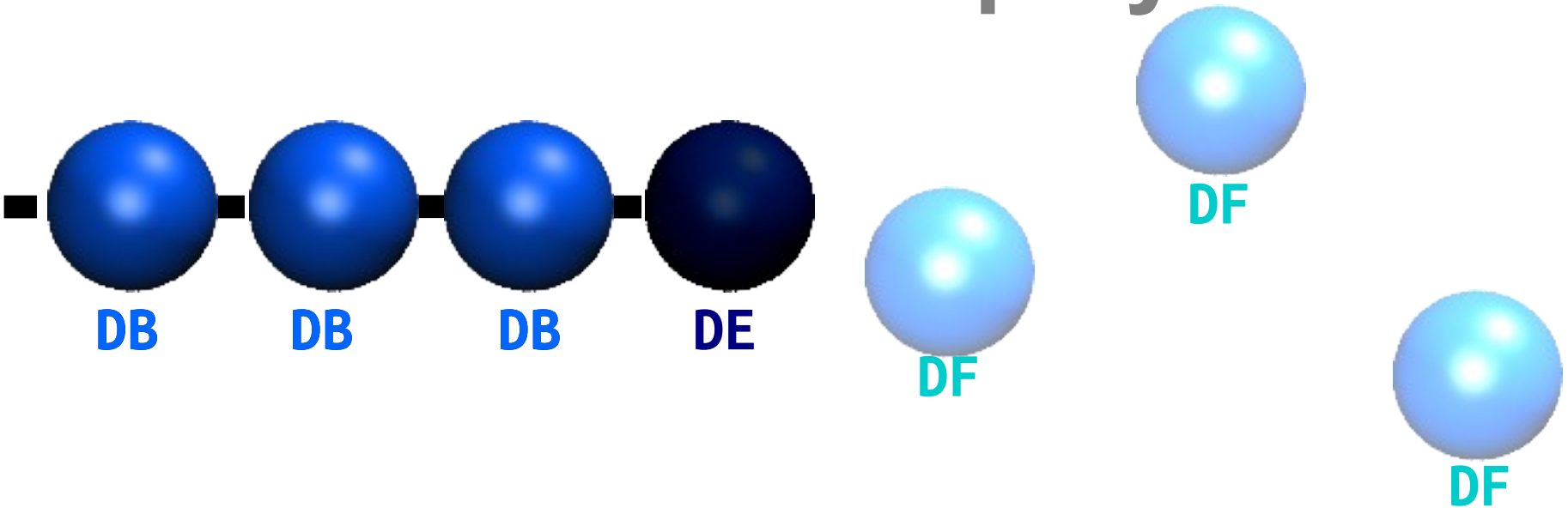
maturation and depolymerization




```
# Transitions 5: Depolymerize ADP-bound ParM at the end (DE)

fix tr6  all  bond/change  100   delay 5                    &
   atoms @atom:DB  @atom:DE                                 &
-> atoms @atom:DE  @atom:DF and bond BREAK
```

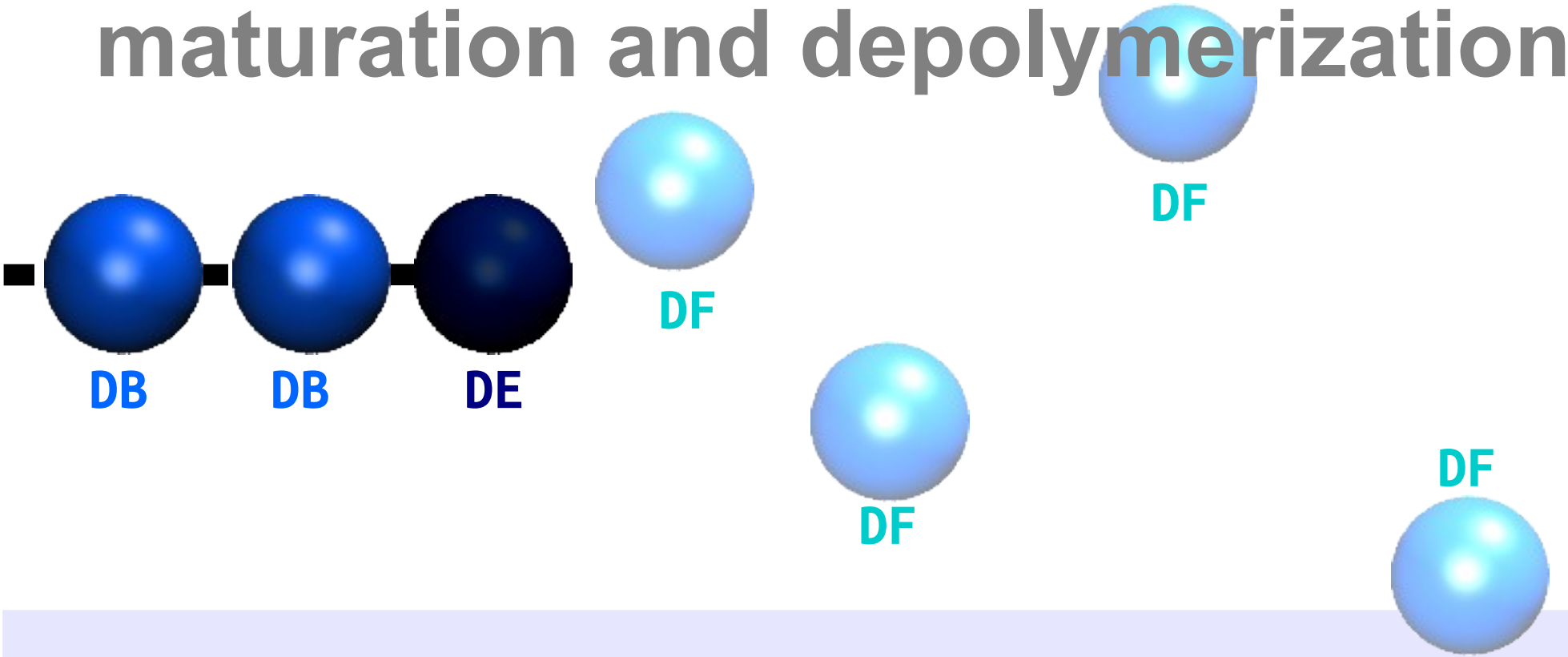
maturation and depolymerization




```
# Transitions 5: Depolymerize ADP-bound ParM at the end (DE)

fix tr6  all  bond/change  100   delay 5                    &
   atoms @atom:DB  @atom:DE                                 &
-> atoms @atom:DE  @atom:DF and bond BREAK
```

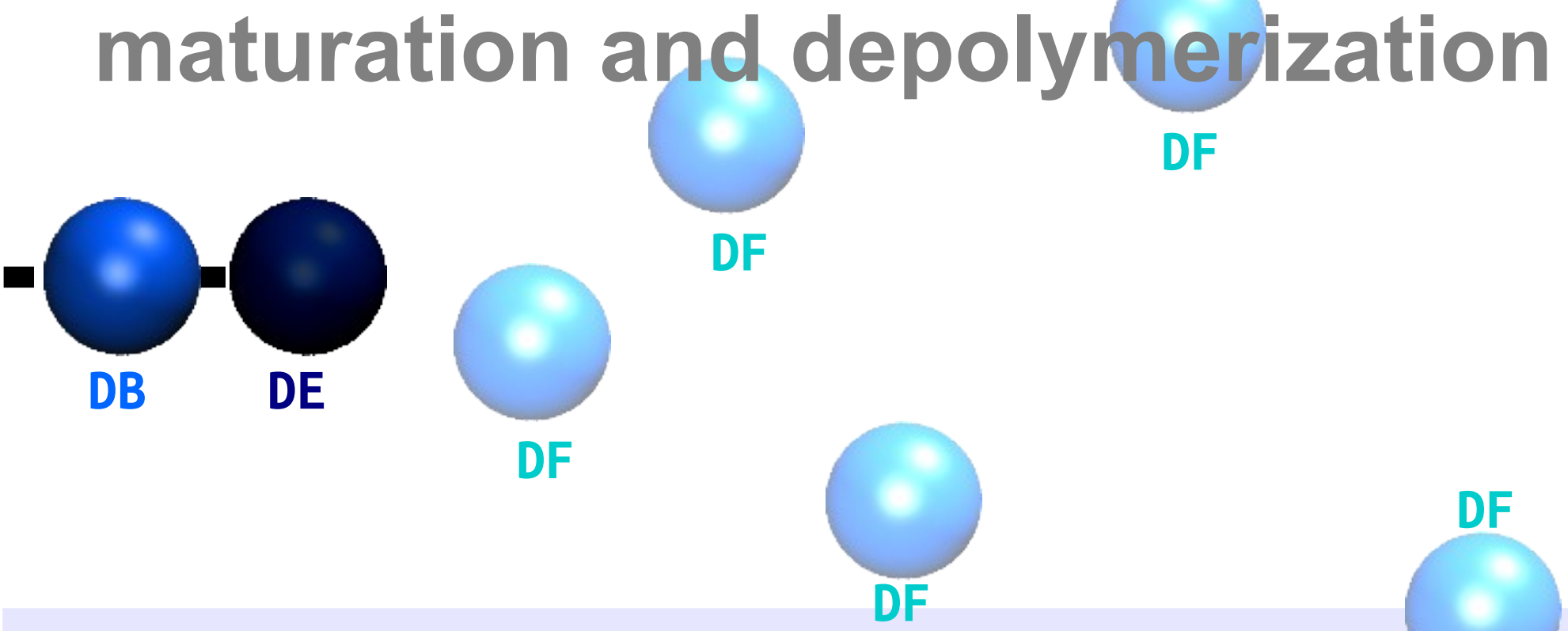
maturation and depolymerization




```
# Transitions 5: Depolymerize ADP-bound ParM at the end (DE)

fix tr6  all  bond/change  100   delay 5                    &
   atoms @atom:DB  @atom:DE                                 &
-> atoms @atom:DE  @atom:DF and bond BREAK
```

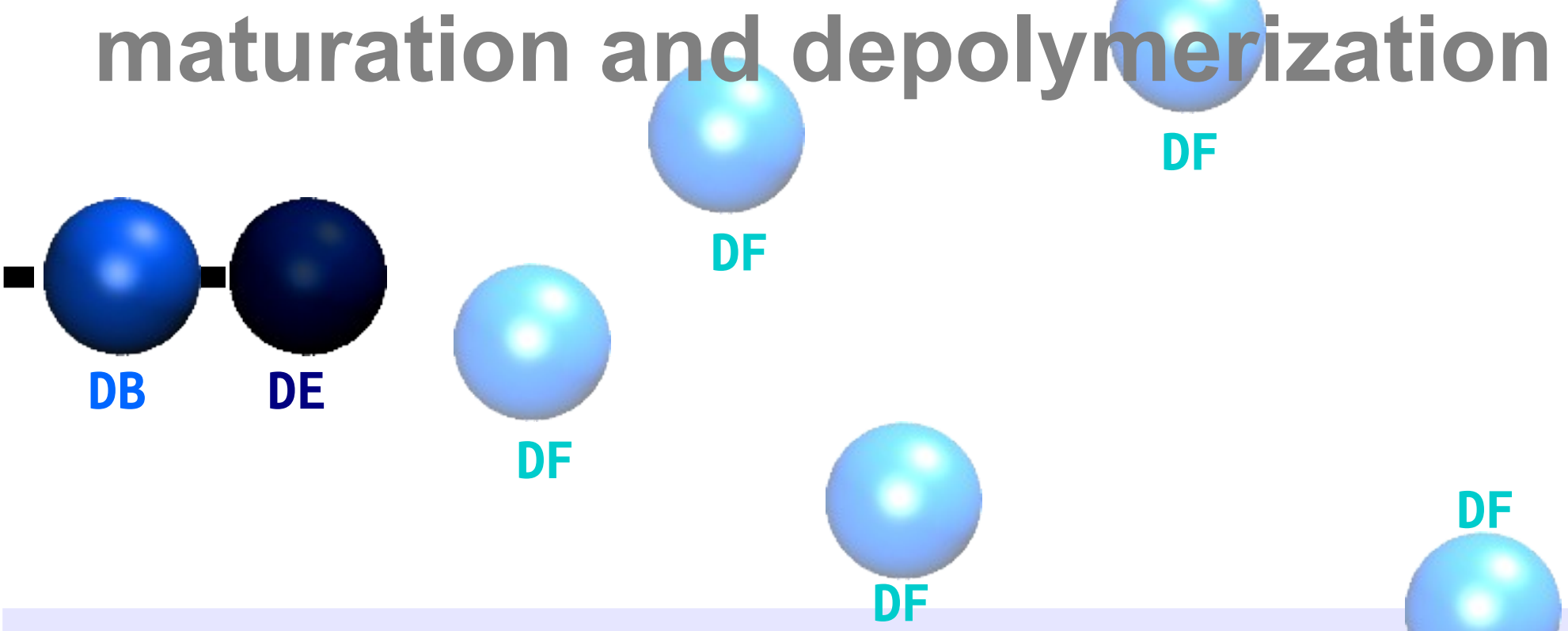
maturation and depolymerization




```
# Transitions 5: Depolymerize ADP-bound ParM at the end (DE)

fix tr6  all  bond/change  100   delay 5                    &
   atoms @atom:DB  @atom:DE                                 &
-> atoms @atom:DE  @atom:DF and bond BREAK
```

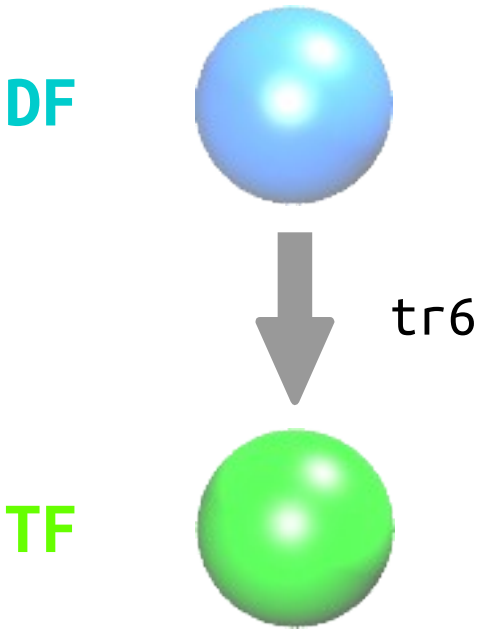
maturation and depolymerization




```
# Transitions 5: Depolymerize ADP-bound ParM at the end (DE)

fix tr6  all  bond/change  100   delay 5                    &
   atoms @atom:DB  @atom:DE                                 &
-> atoms @atom:DE  @atom:DF and bond BREAK
```

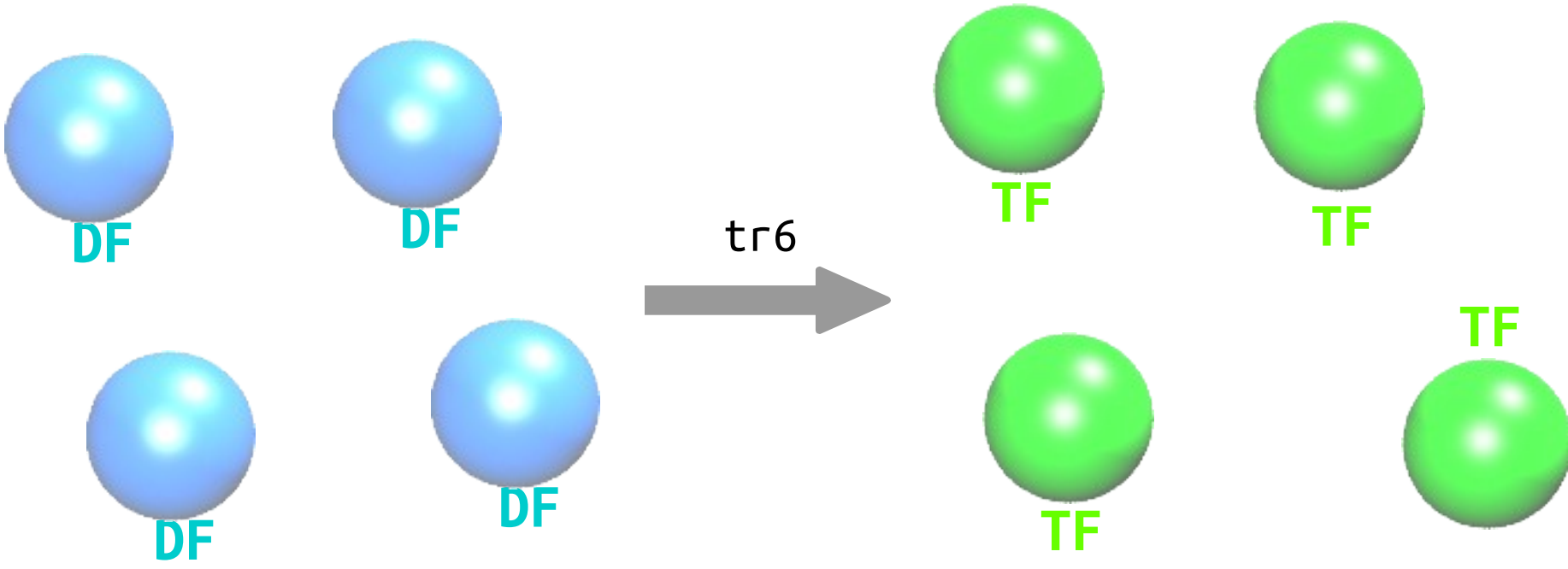
maturation and depolymerization




```
# Transition 6: Recycle ATP -> ADP  (bound to ParM)

fix tr6  all  atom/change  100   delay 6                    &
   atom @atom:DF and prob 0.0015  ->  atom @atom:TF
```

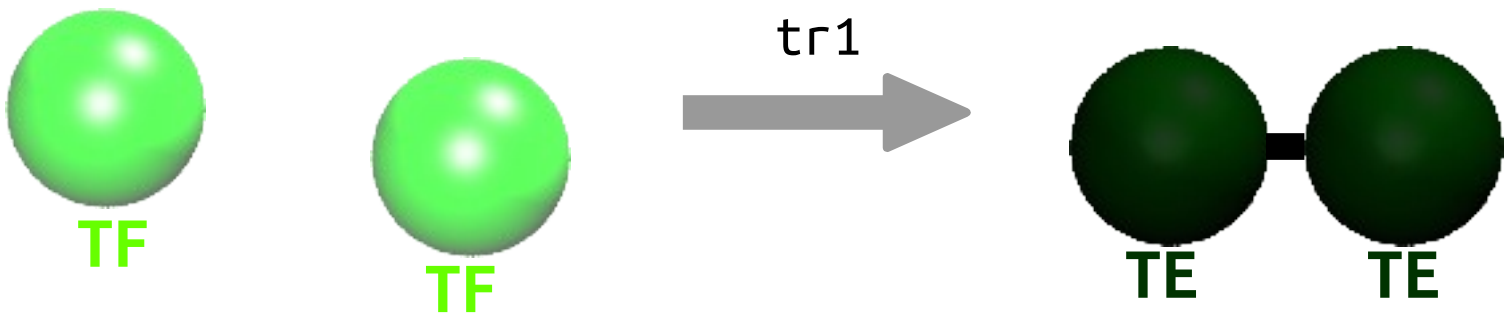
maturation and depolymerization




```
# Transition 6: Recycle ATP -> ADP  (bound to ParM)

fix tr6  all  atom/change  100   delay 6                    &
   atom @atom:DF and prob 0.0015  ->  atom @atom:TF
```

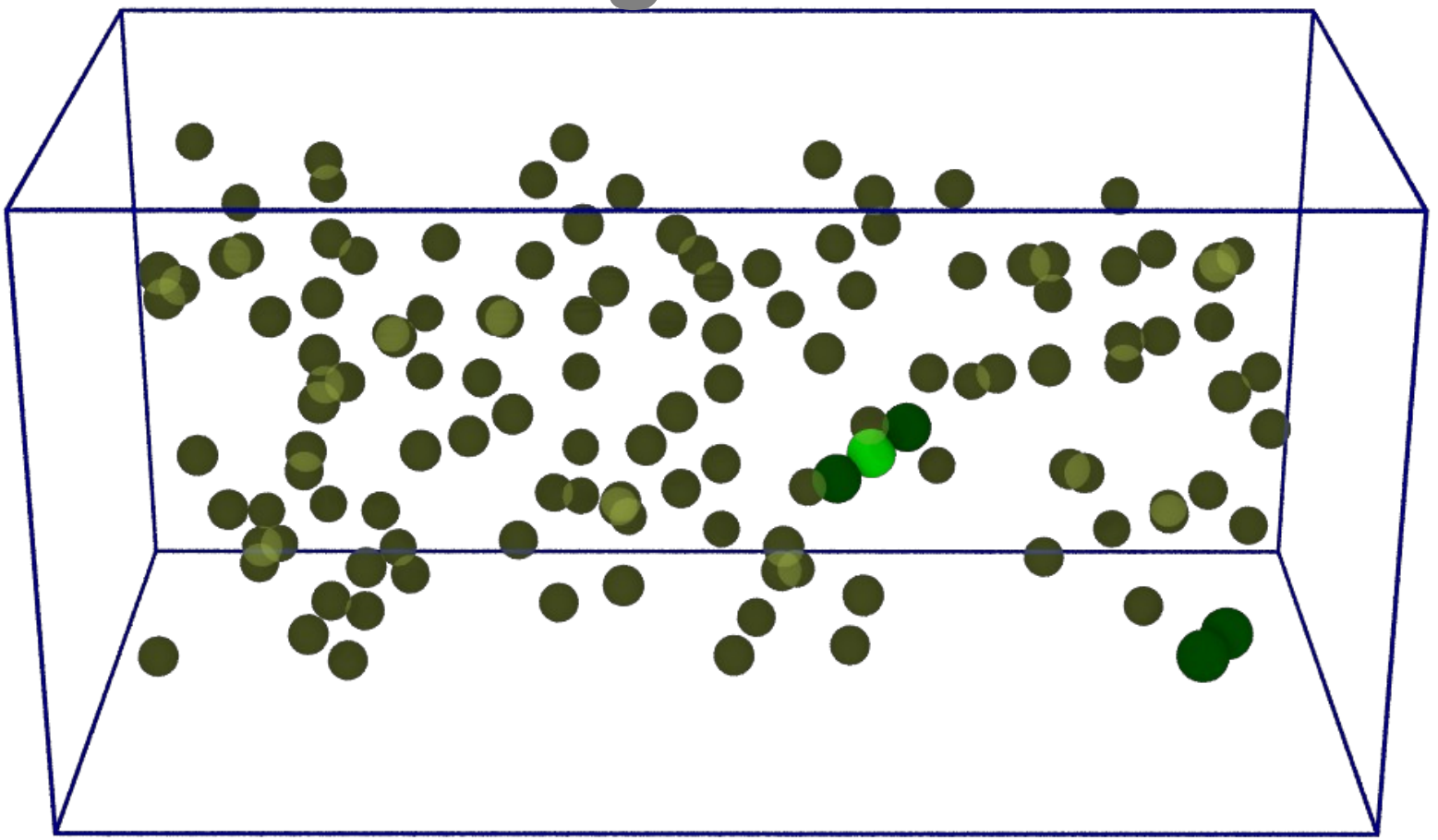
Example: Dynamic Instabilty of ParM




```
# Transition 1: Create a polymer (a dimer)

fix tr1  all  bond/new     100   delay 1                      &
  atoms @atom:TF @atom:TF and distance <= 7.1 and prob 0.1 &
-> atoms @atom:TE @atom:TE and bond @bond:F
```

slow growth...

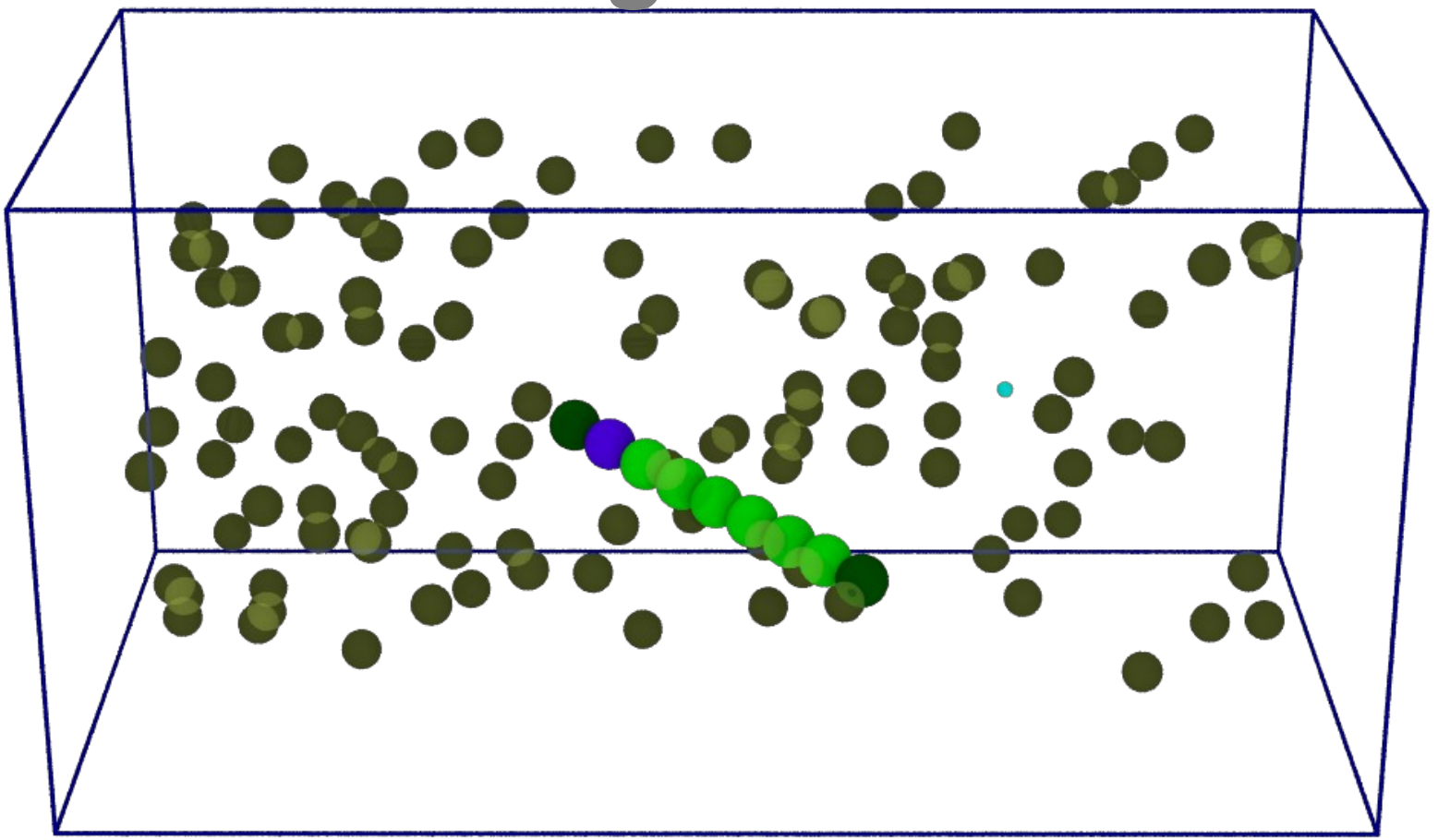


ParM + ATP

ParM + ADP

Garner, …, Mullins, Science (2004)

slow growth...

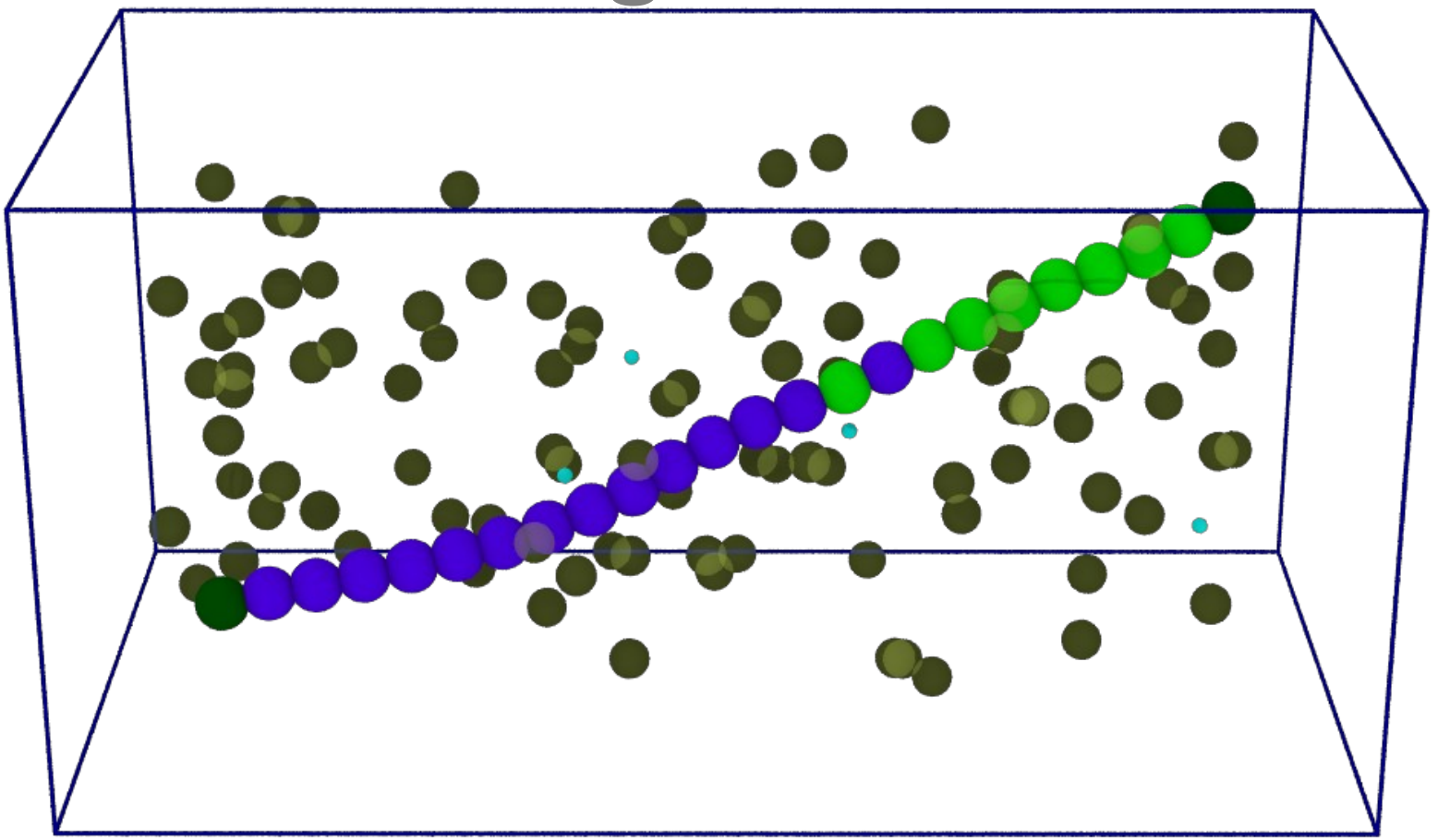


ParM + ATP

ParM + ADP

Garner, …, Mullins, Science (2004)

slow growth...

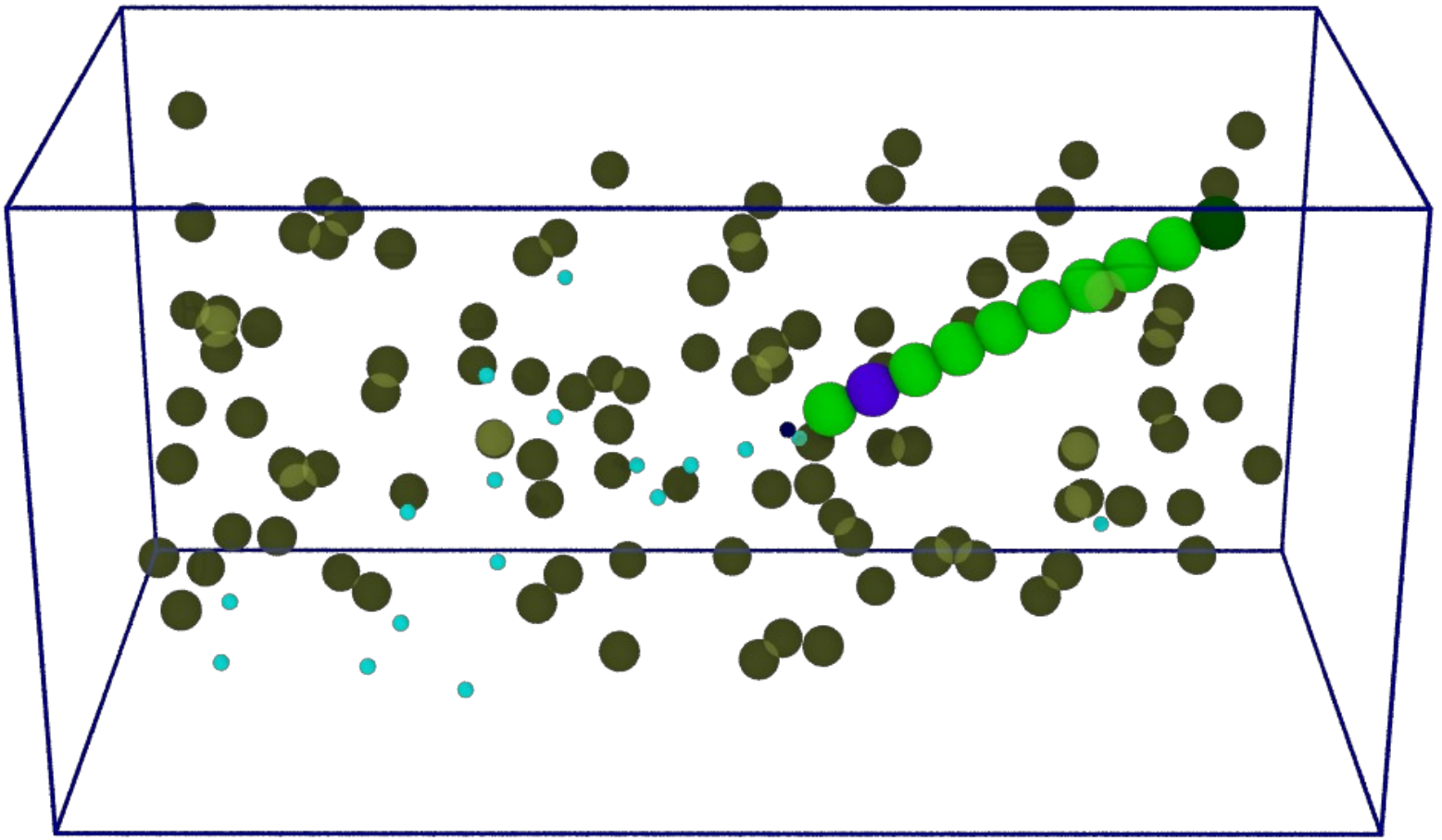


ParM + ATP

ParM + ADP

Garner, …, Mullins, Science (2004)

sudden collapse



ParM + ATP

ParM + ADP

Garner, …, Mullins, Science (2004)

repeat...

If you have time, see the youtube video at:

https://www.youtube.com/watch?v=EEbt07vZHew