rule-based (RB) pratical #1

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What we need to start

www.di.ens.fr/~feret/teaching/2014-2015/master_AIV

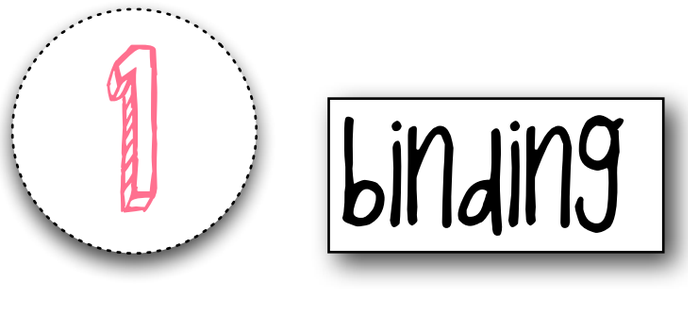
be sure to use the manual!

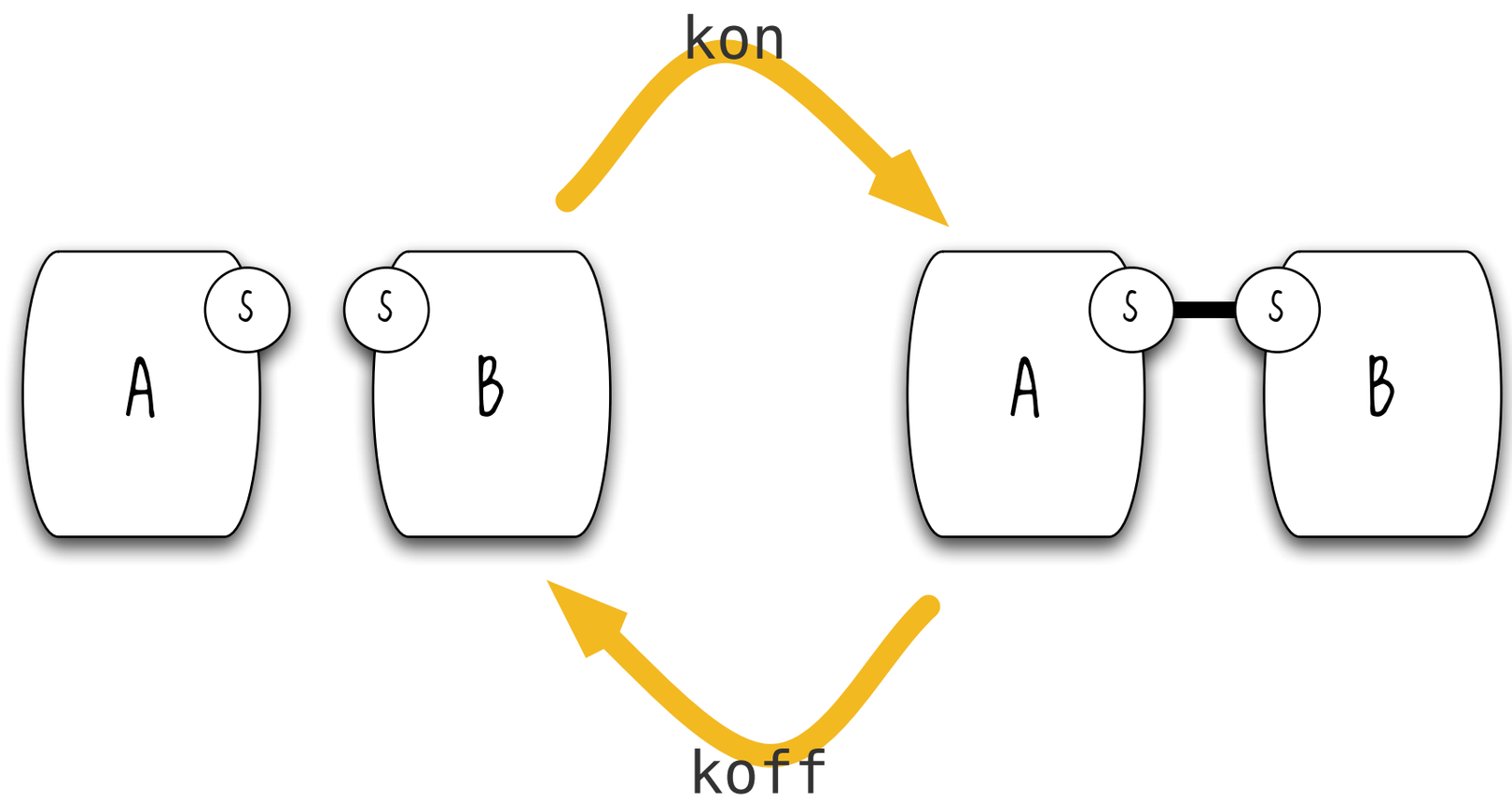
first steps

```
open the terminal!
```

```
in the terminal go to the directory where KaSim is
do > ls -lt
```

```
change ownership of KaSim_3.5_mac_OSX_10.10
> chmod u+x KaSim_3.5_mac_OSX_10.10
> mv KaSim_3.5_mac_OSX_10.10 Kasim
> ./Kasim -version
```


1
binding




```
A(s), B(s) -> A(s!0), B(s!0) @ 0.00001
A(s!0), B(s!0) -> A(s), B(s) @ 0.1
```

create the file AB.ka in an editor (emacs, textedit in text mode, textwrangler, etc)

model

```
%agent: A(s)
%agent: B(s)

A(s), B(s) -> A(s!0), B(s!0) @ 0.00001
A(s!0), B(s!0) -> A(s), B(s) @ 0.1

%init: 1000 A(s)
%init: 1000 B(s)

%obs: 'AB' A(s!1), B(s!1)
```

command line

```
sh>./KaSim -i AB.ka -e 2000 -p 100
```

plot

```
sh>./plot data.out &
```

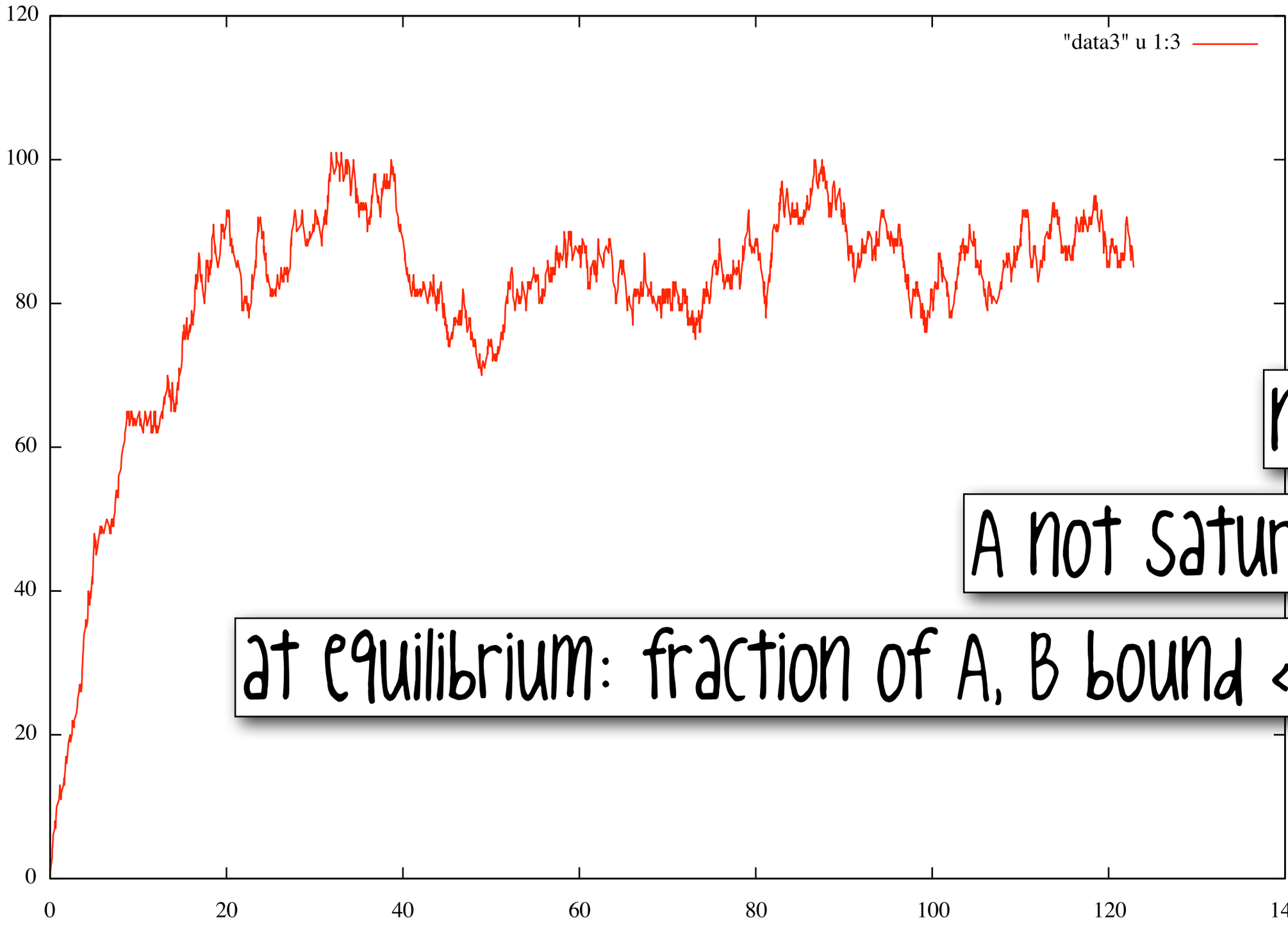
data.out

data.out

```
# time E 'AB'
 0.000000E+00 0 0.000000E+00
 1.536270E+00 20 1.400000E+01
 3.248637E+00 40 2.400000E+01
 4.857524E+00 60 3.000000E+01
 5.800390E+00 80 4.200000E+01
 7.642658E+00 100 5.200000E+01
 8.799027E+00 120 4.800000E+01
 .....
```

using gnuplot

```
gnuplot> plot "data.out" using 1:3 with lines
```



noisy

A not saturated

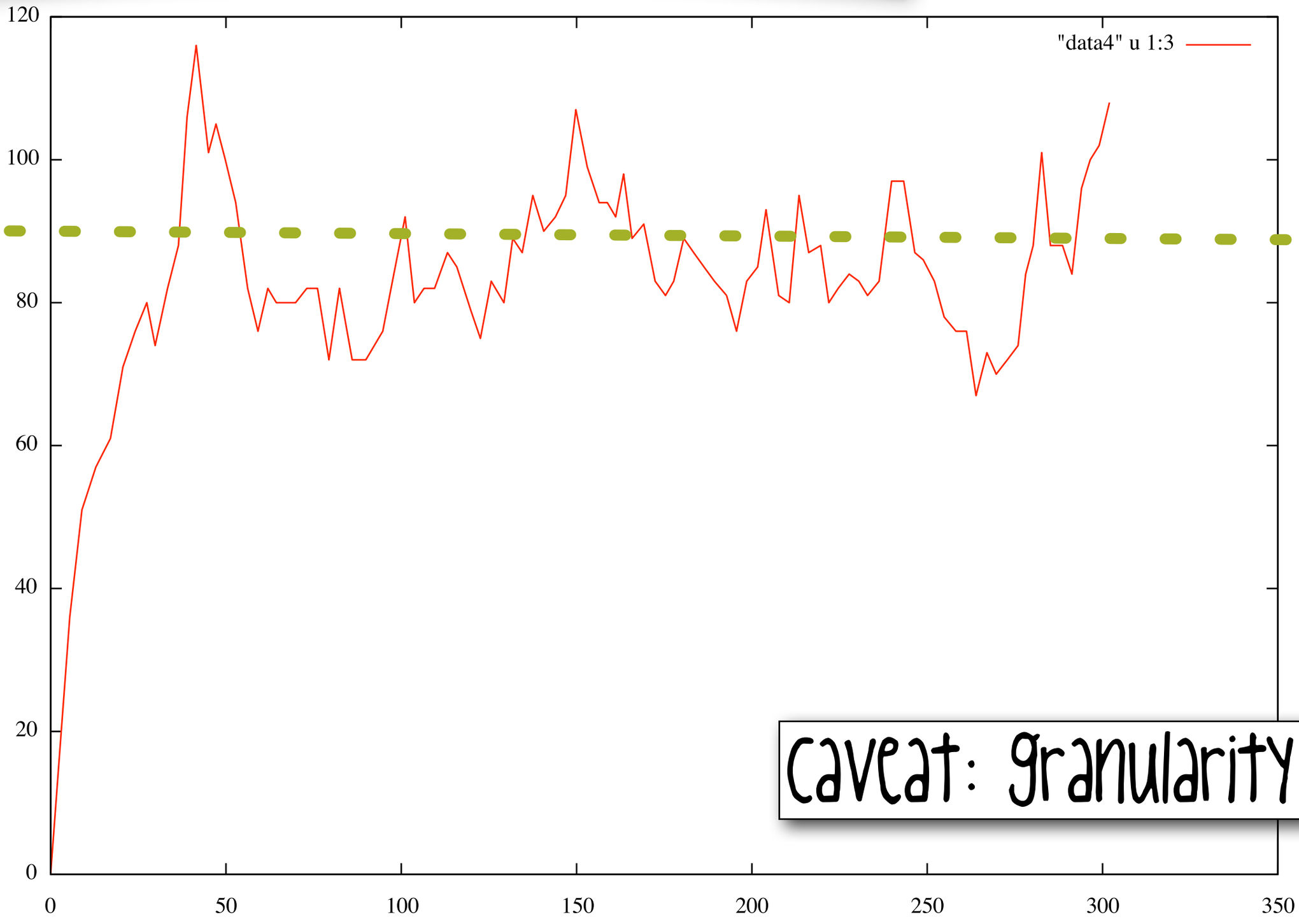
at equilibrium: fraction of A, B bound < 10%

What is the time to equilibrium roughly?

how does one define equilibrium?

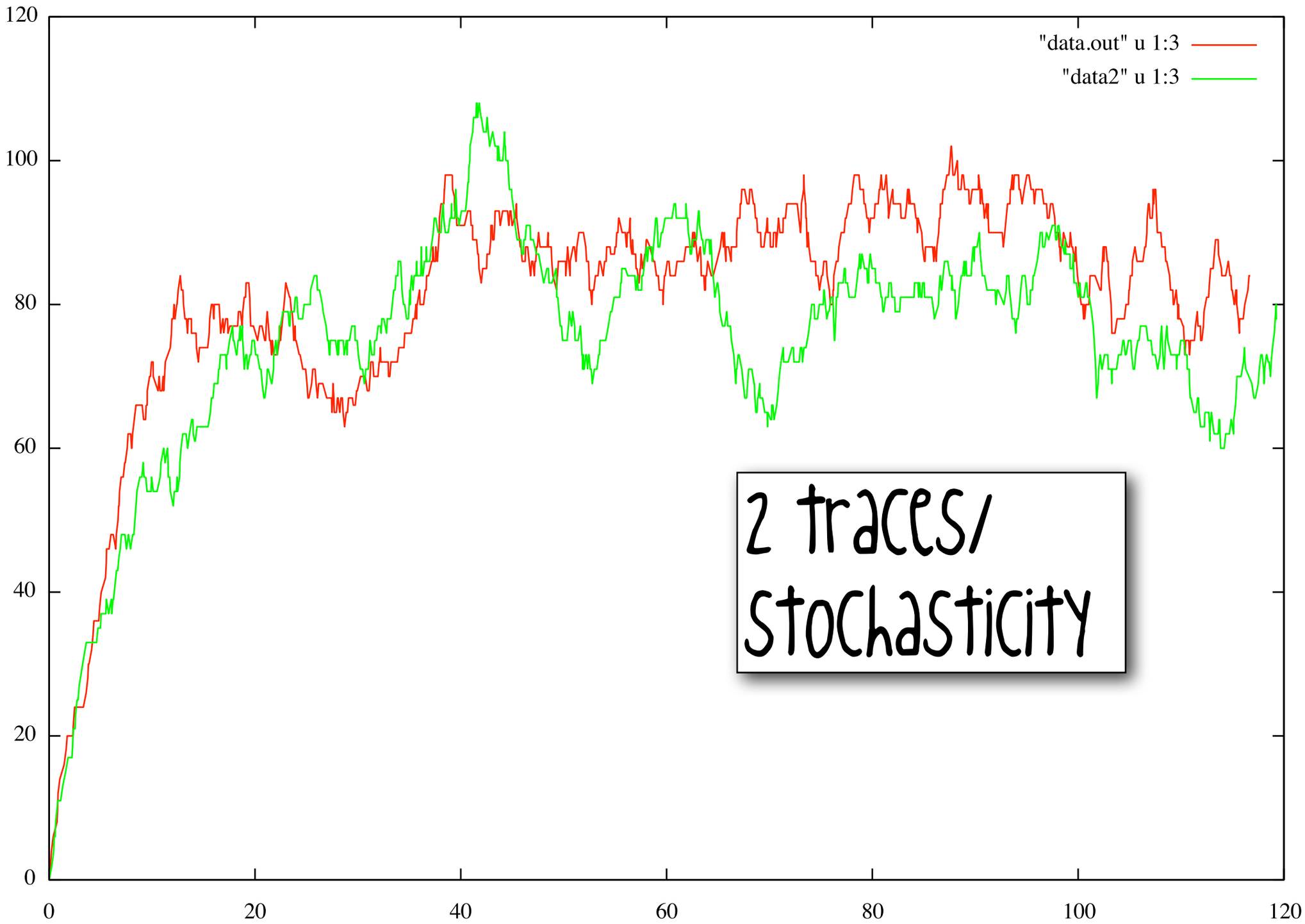
run same for longer

```
KaSim -i AB.ka -t 300 -p 100 -o yourname
```



caveat: granularity -p

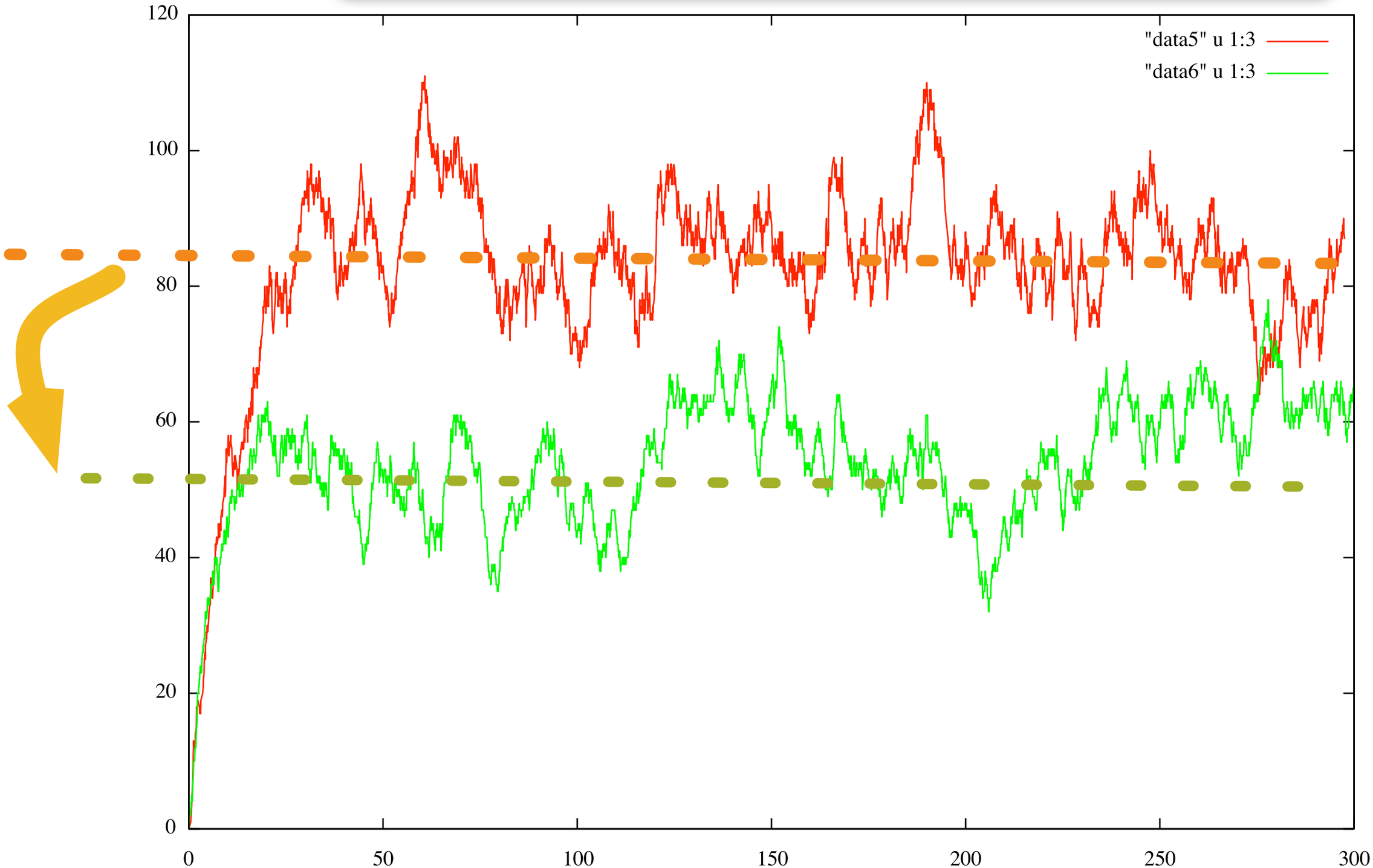
run the model a second time in the same conditions



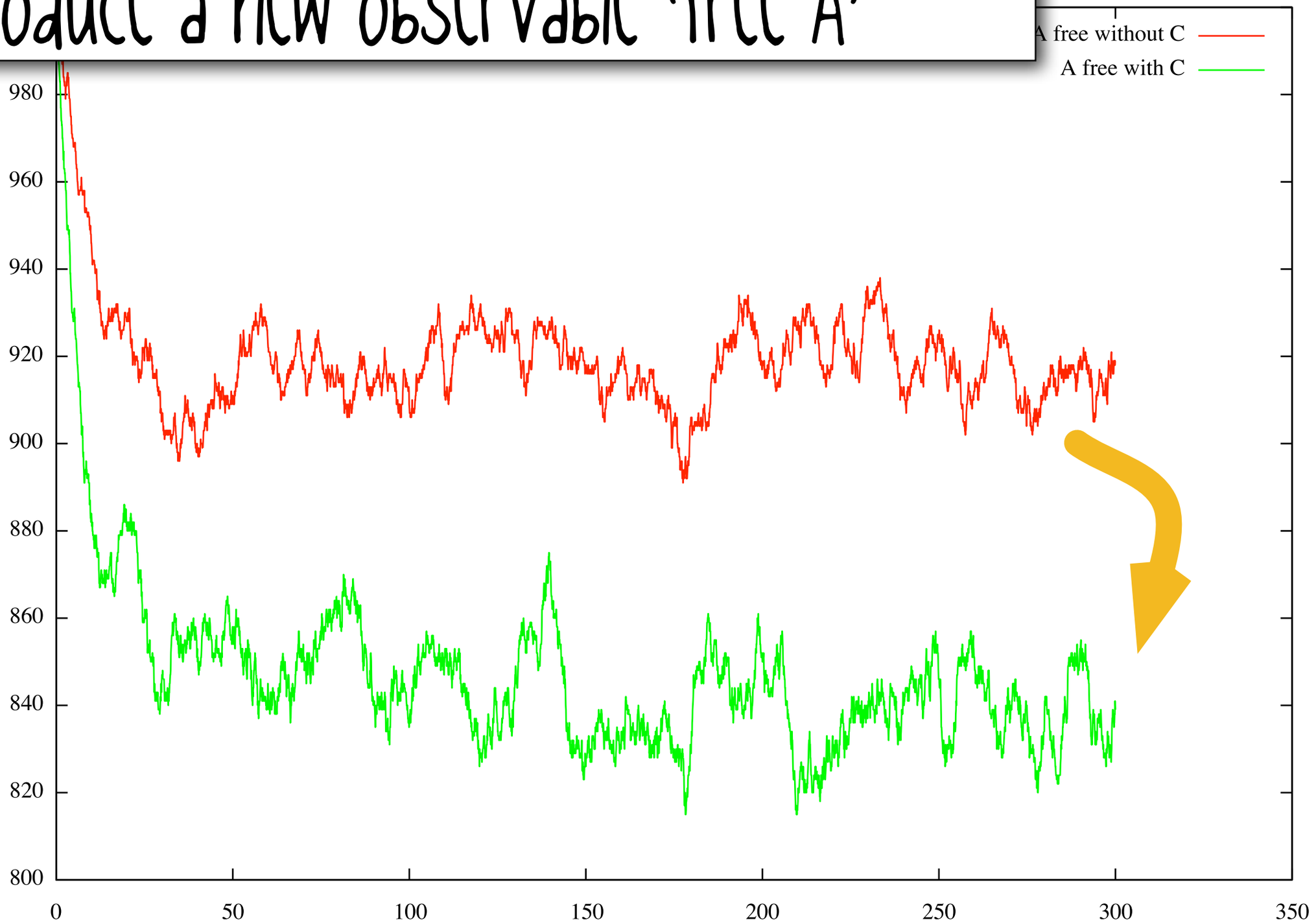
2 traces/
stochasticity

conflict introduce agent C that also binds A

the number of AB dimers goes down??



With another (1000) C to bind A - we introduce a new observable 'free A'



is A more saturated? Yes about 20%

2

other games we can play

decrease/increase k_off

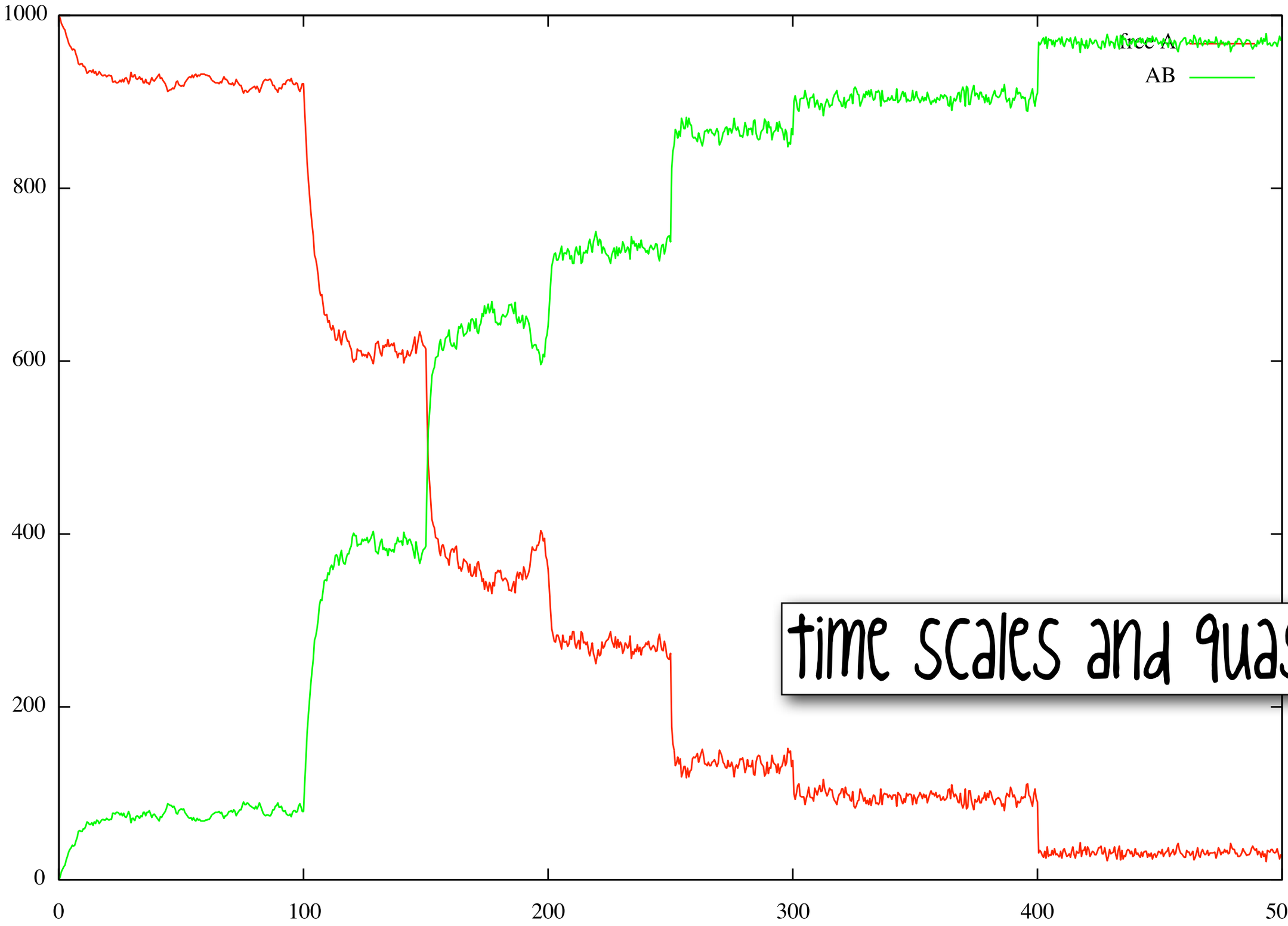
decrease/increase k_on

using mods!

```
%mod: [T] > 100 do 'assoc' := 0.0001
```

```
%mod: [T] > 200 do 'assoc' := 0.001
```

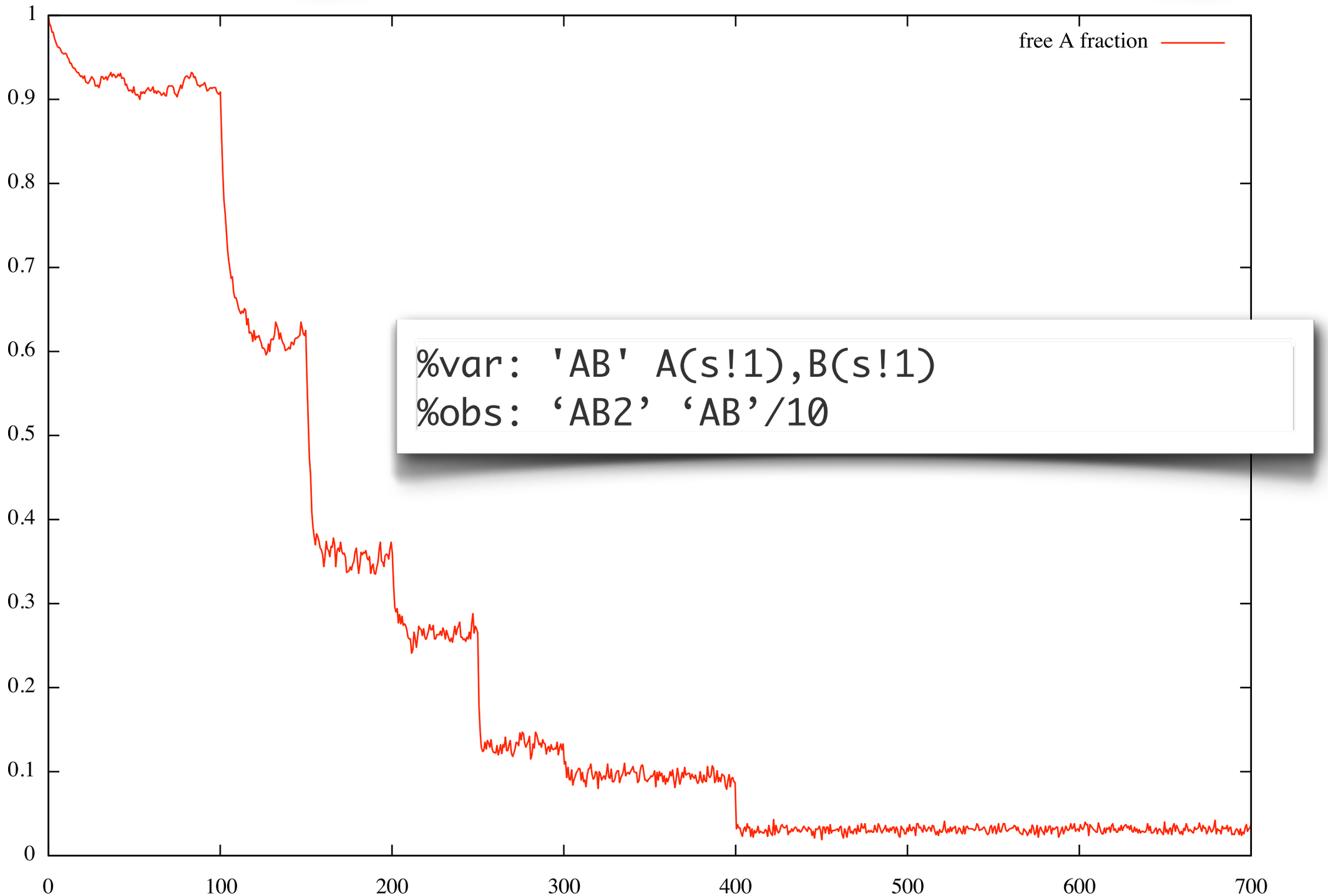
```
etc ...
```


1000
800
600
400
200
0
0
100
200
300
400
500
free A
AB
time scales and quasi-E9

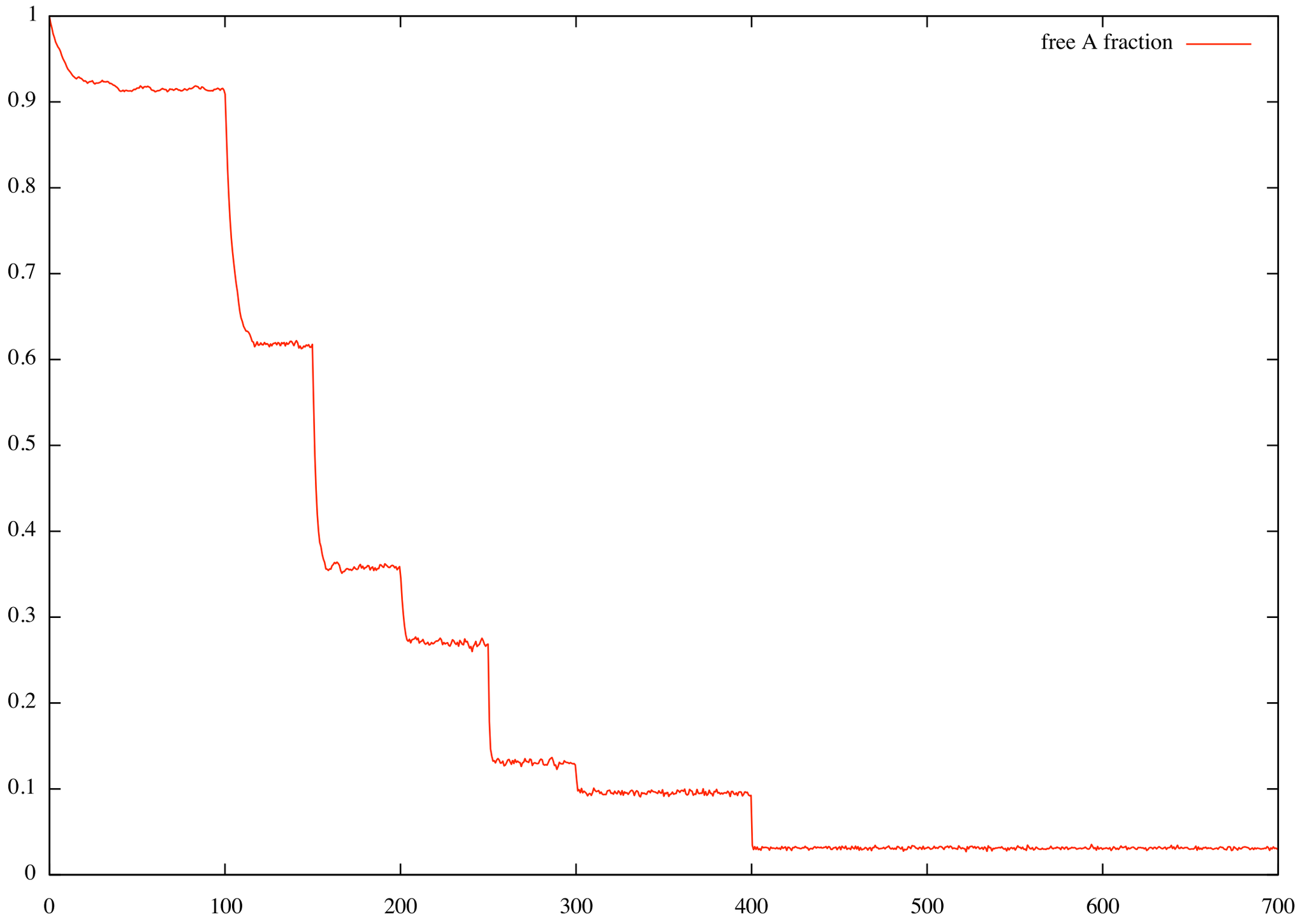
```
%agent: A(s)
%agent: B(s)

%var: 'vol' 1
%var: 'nA'  1000 * 'vol'
%var: 'nB'  1000 * 'vol'

%init: 'nA' A(s)
%init: 'nB' B(s)

%var: 'fast' 10
%var: 'medium' 1
%var: 'slow' 0.1
%var: 'BND' 0.00001 / 'vol'
%var: 'BRK' 0.1
%var: 'MOD' 0.1

'assoc'  A(s), B(s) -> A(s!0), B(s!0) @ 'BND' # * 'fast'
'dissoc' A(s!0), B(s!0) -> A(s), B(s) @ 'BRK' # * 'slow'

%var: 'free As' A(s)
%obs: 'free A fraction' 'free As' / 'nA'

%mod: [T] > 100 do 'assoc' := 10 * 'BND'
%mod: [T] > 150 do 'assoc' := 50 * 'BND'
%mod: [T] > 200 do 'assoc' := 100 * 'BND'
%mod: [T] > 250 do 'assoc' := 500 * 'BND'
%mod: [T] > 300 do 'assoc' := 1000 * 'BND'
%mod: [T] > 400 do 'assoc' := 10000 * 'BND'
```

can plot the free fraction directly

```
%obs: 'free A fraction' 'free As' / 'nA'
```




```
%var: 'AB' A(s!1),B(s!1)
%obs: ‘AB2’ ‘AB’/10
```


free A fraction
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0
100
200
300
400
500
600
700

rescale!

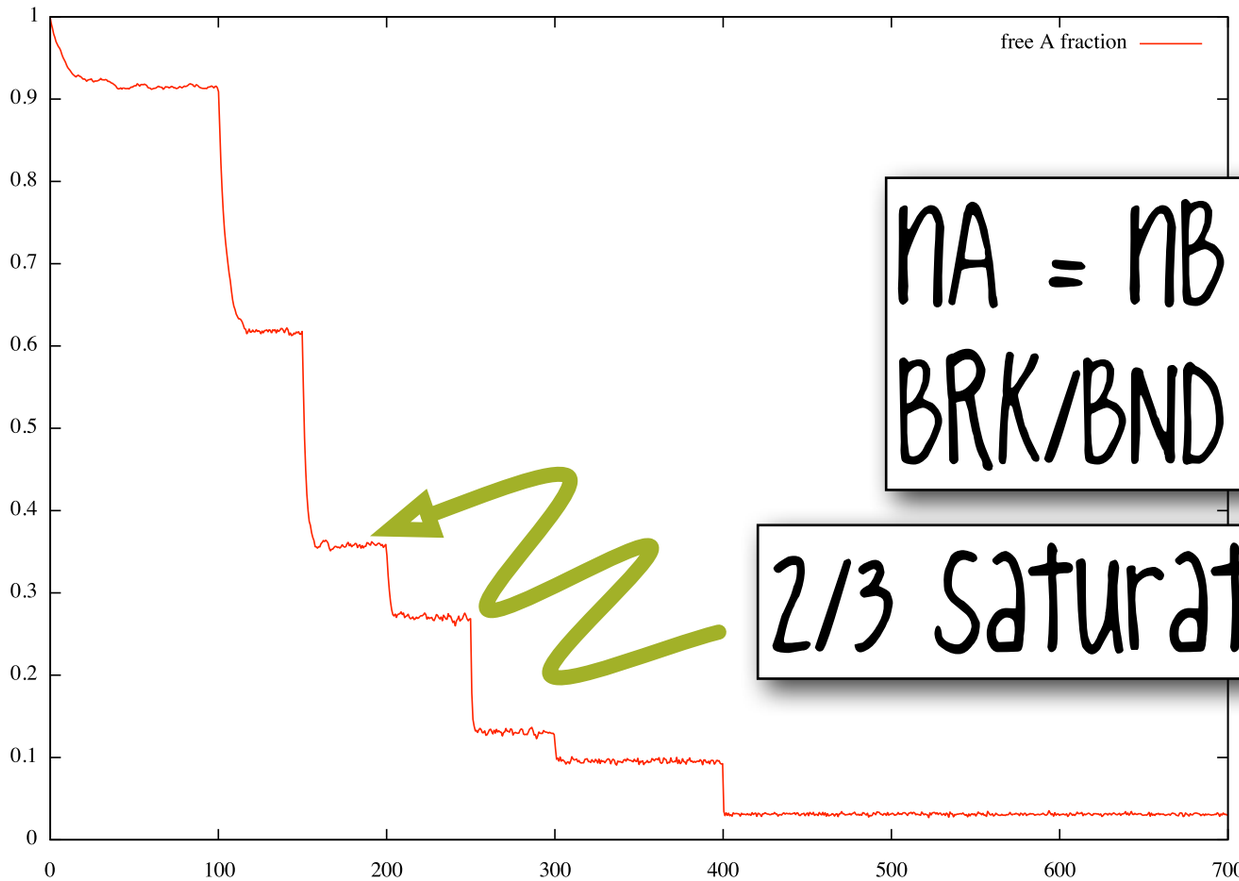
vol = 10

```
%var: 'vol' 1
%var: 'nA'  1000 * 'vol'
%var: 'nB'  1000 * 'vol'

%init: 'nA' A(s)
%init: 'nB' B(s)
```

```
%var: 'BND' 0.00001 / 'vol'
%var: 'BRK' 0.1

'assoc'  A(s), B(s) -> A(s!0), B(s!0) @ 'BND'
'dissoc' A(s!0), B(s!0) -> A(s), B(s) @ 'BRK'
```

```
%mod: [T] > 100 do 'assoc' := 10 * 'BND'
%mod: [T] > 150 do 'assoc' := 50 * 'BND'
%mod: [T] > 200 do 'assoc' := 100 * 'BND'
%mod: [T] > 250 do 'assoc' := 500 * 'BND'
%mod: [T] > 300 do 'assoc' := 1000 * 'BND'
%mod: [T] > 400 do 'assoc' := 10000 * 'BND'
```

this curve solves Kd(saturation)



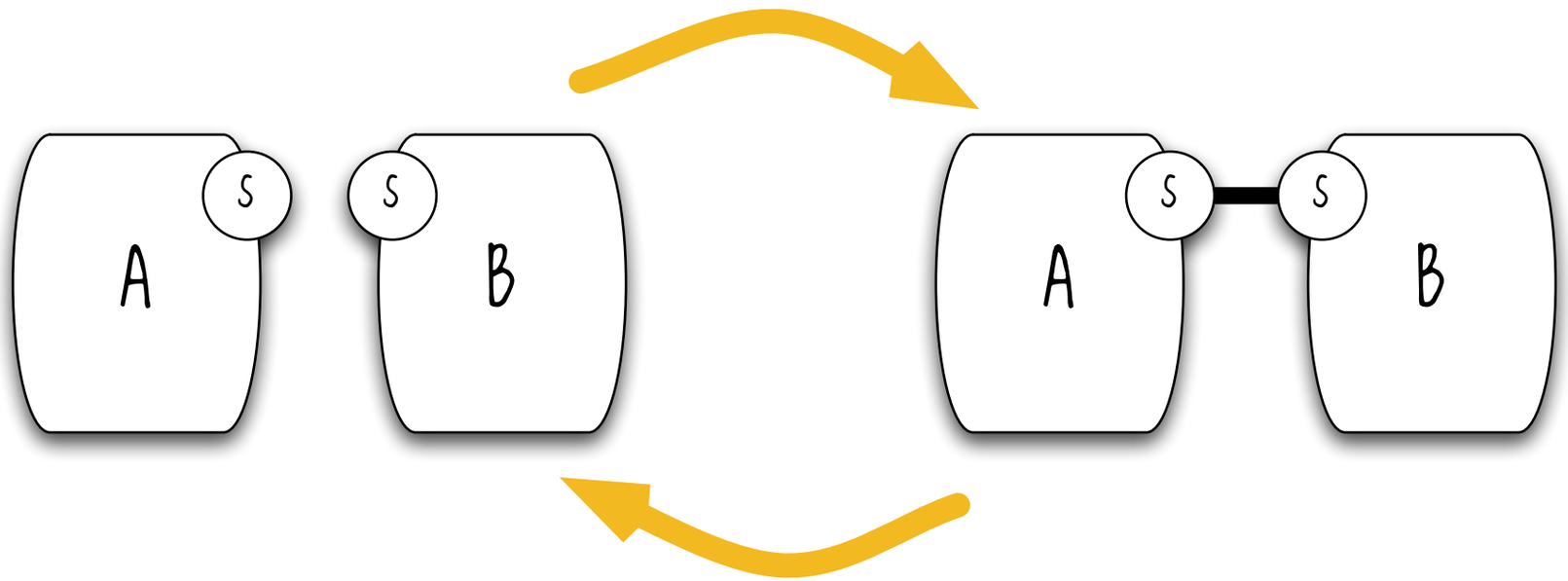
nA = nB = 1000 Vol

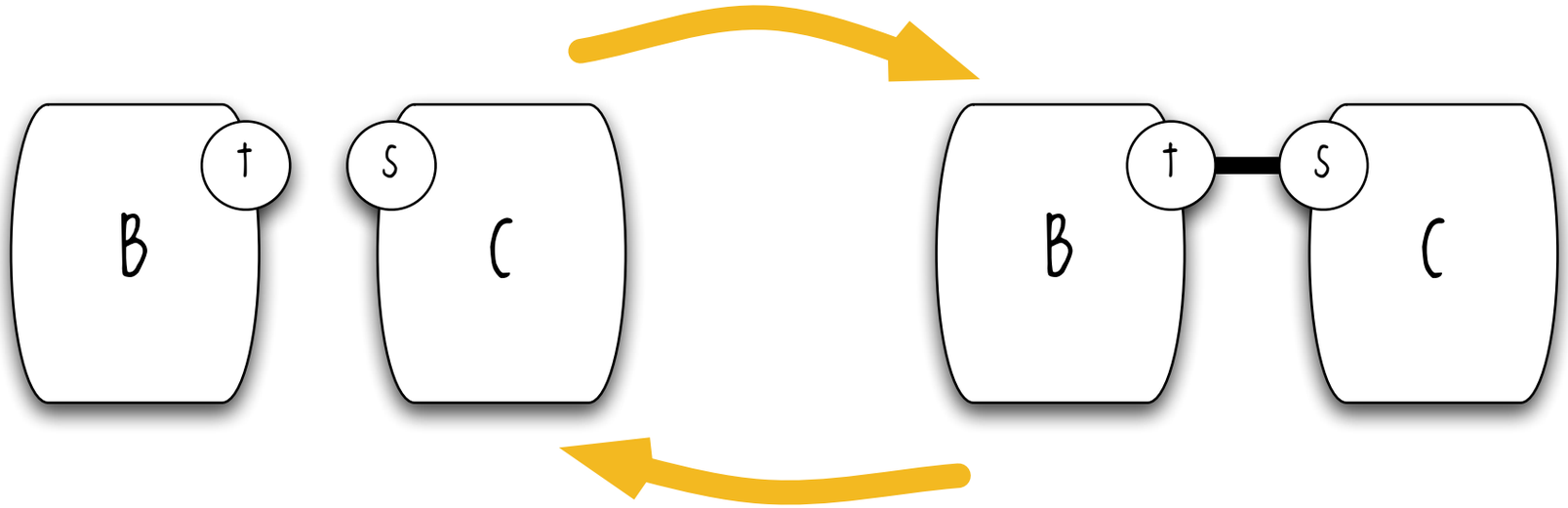
BRK/BND = 5000 Vol

2/3 Saturation

3

independent binding


A
S
B
S
A
S
S
B


B
†
C
S
B
†
S
C

getting organized

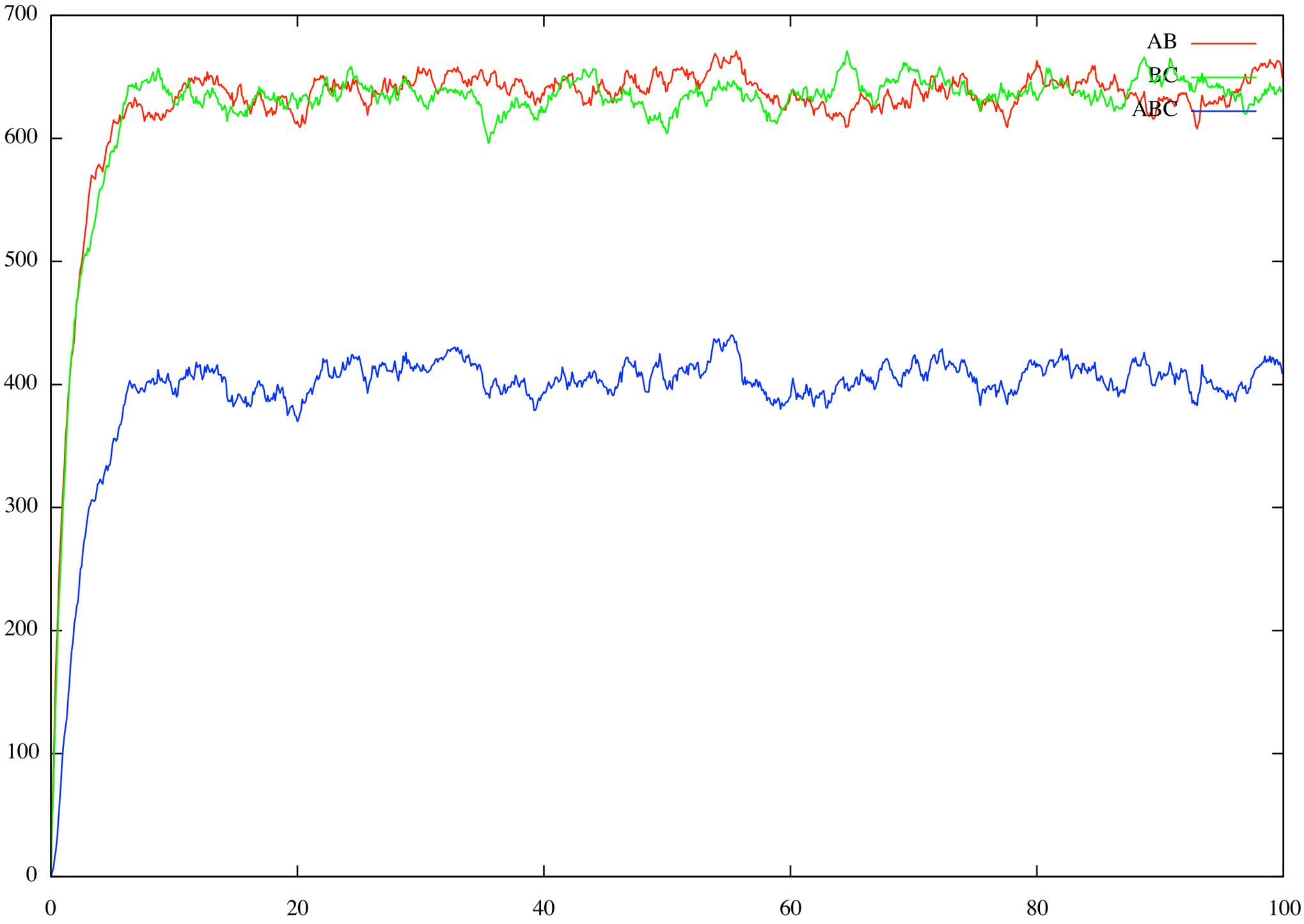
```
KaSim -i ABC.ka -t 100 -p 1000 -d ABCdata -o data1
```

run this model with medium sticky, 2/3 saturation

everything as in the preceding AB example

```
%var: 'BND' 0.0005 / 'vol'
```

plot AB, BC, and ABC


700
600
500
400
300
200
100
0
0
20
40
60
80
100
AB
BC
ABC

```
#%var: 'nB'  1000 * 'vol'
%var: 'nB'  0 * 'vol'
%var: 'nC'  1000 * 'vol'

%init: 'nA' A(s)
%init: 'nB' B(s)
%init: 'nC' C(s)

%var: 'BND' 0.0005 / 'vol'
%var: 'BRK' 0.1

'assocAB'  A(s), B(s) -> A(s!0), B(s!0) @ 'BND'
'dissocAB' A(s!0), B(s!0) -> A(s), B(s) @ 'BRK'
'assocBC'  B(t), C(s) -> B(t!0), C(s!0) @ 'BND'
'dissocBC' B(t!0), C(s!0) -> B(t), C(s) @ 'BRK'
```

```
%obs: 'AB' B(s!_)
%obs: 'BC' B(t!_)
%obs: 'ABC' B(s!_,t!_)
%obs: 'B' B()
%obs: 'ABC fraction' 'ABC' / 'B'

%var: 'INJ' 0.1 * 'vol'
'inject' -> B(s,t) @ 'INJ'

%mod: [T] > 60000 do 'inject' := 0
```

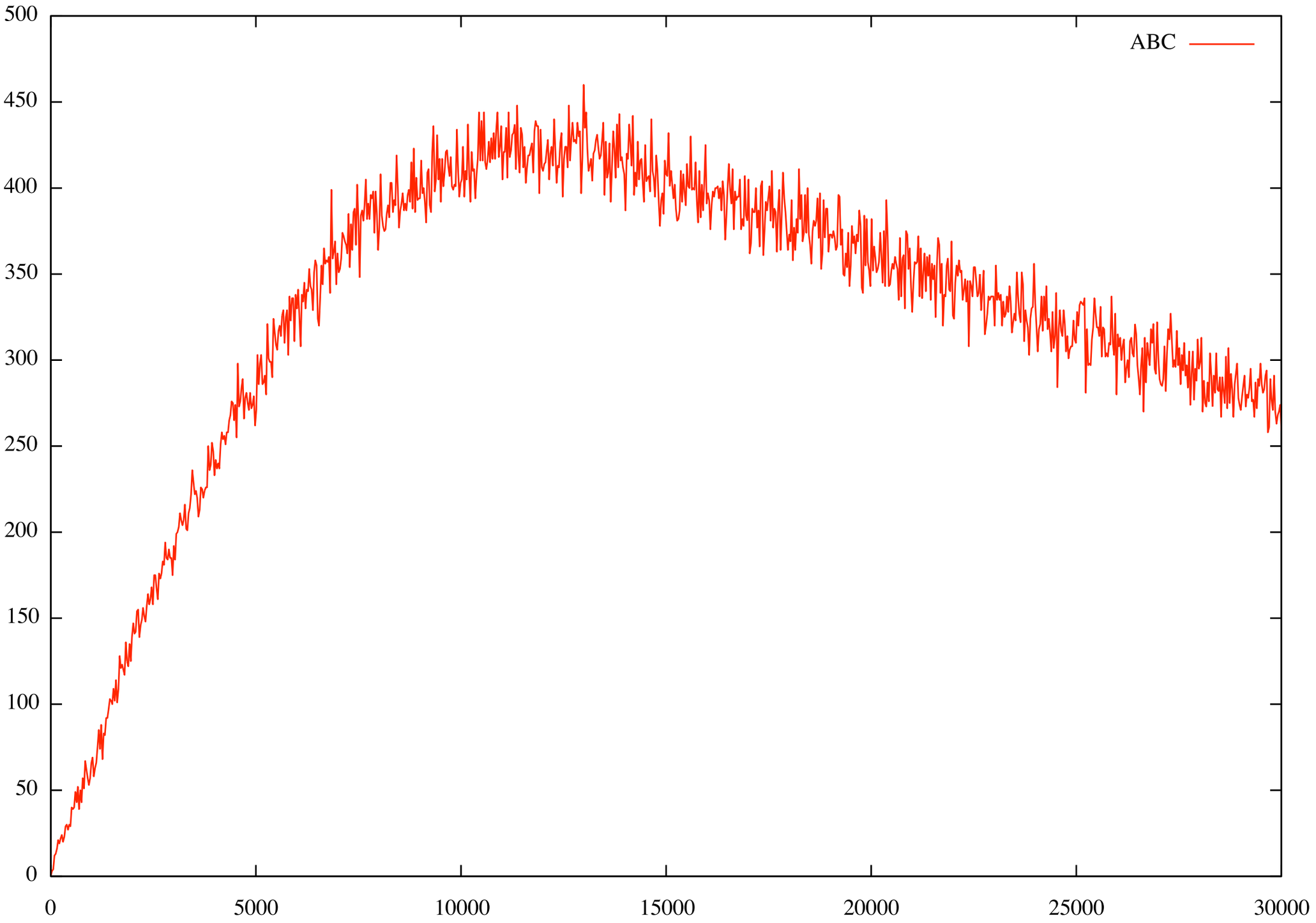
same thing but gradually injecting B's

```
%var: 'INJ' 0.1 * 'vol'
'inject' -> B(s,t) @ 'INJ'
```

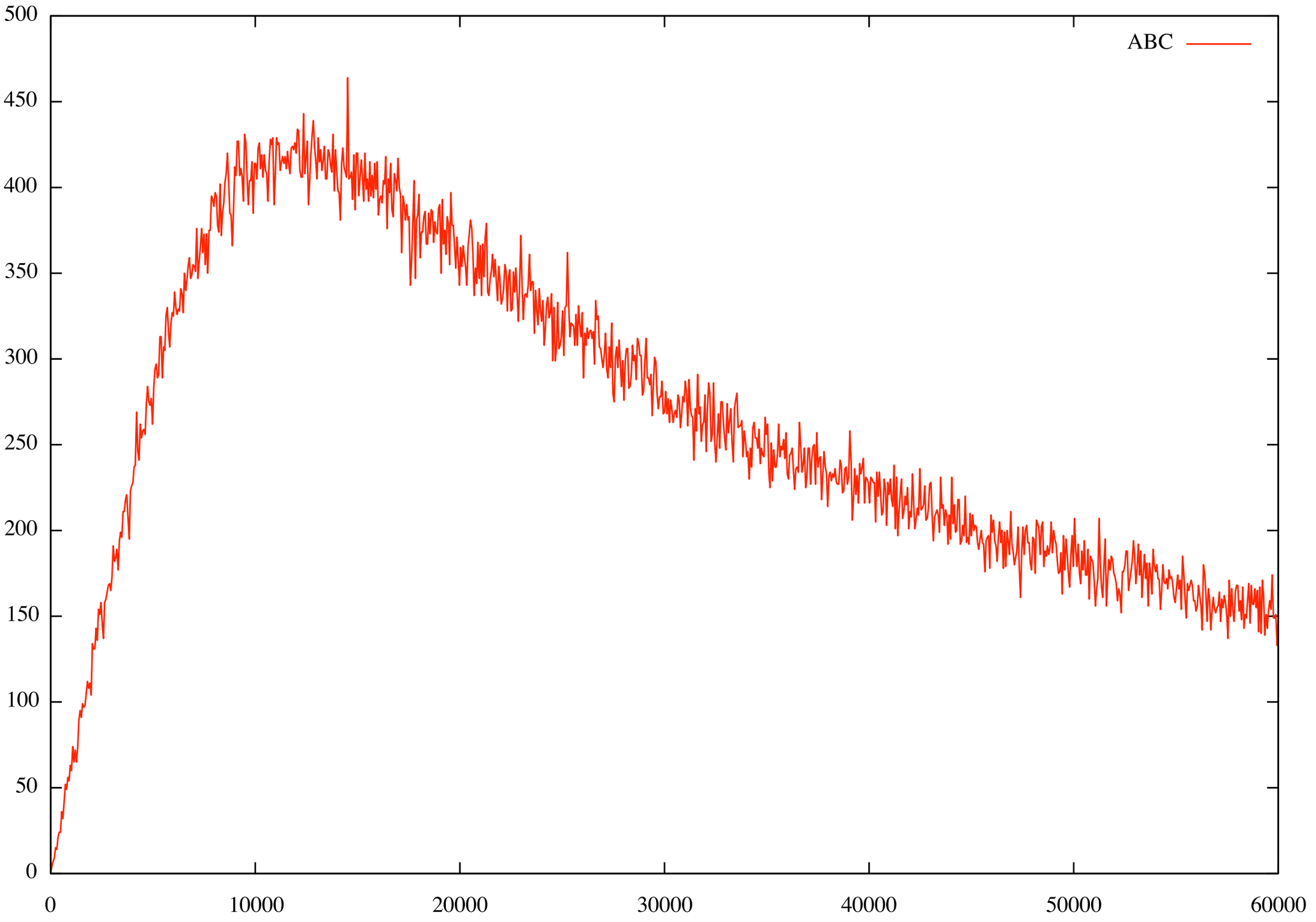
how fast can you inject B's?

concept of quasi-equilibrium

non monotonic!

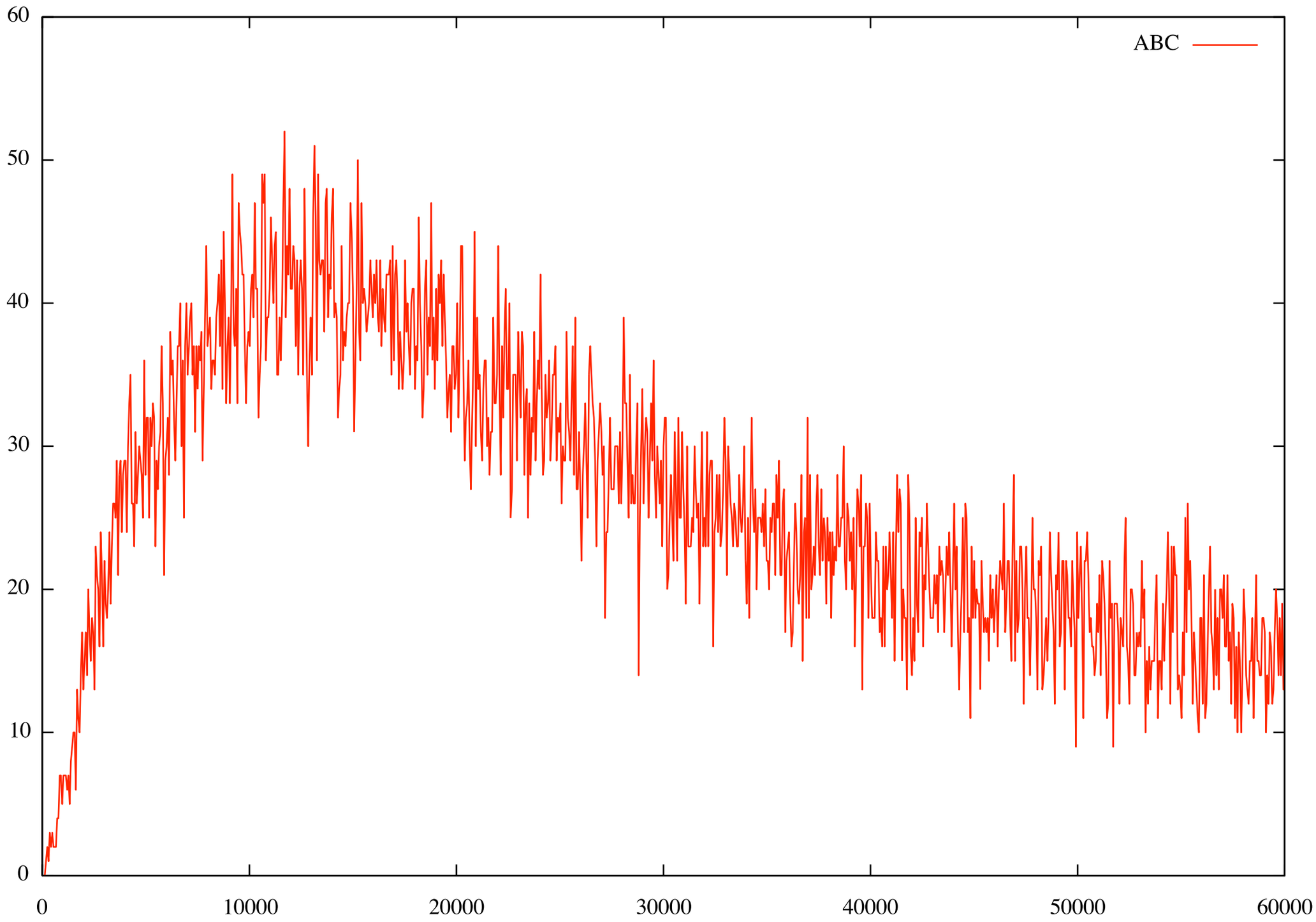


Vol = 1 total time = 3000



Vol = 1 total time = 6000

tip: use smaller vols if simulation too slow

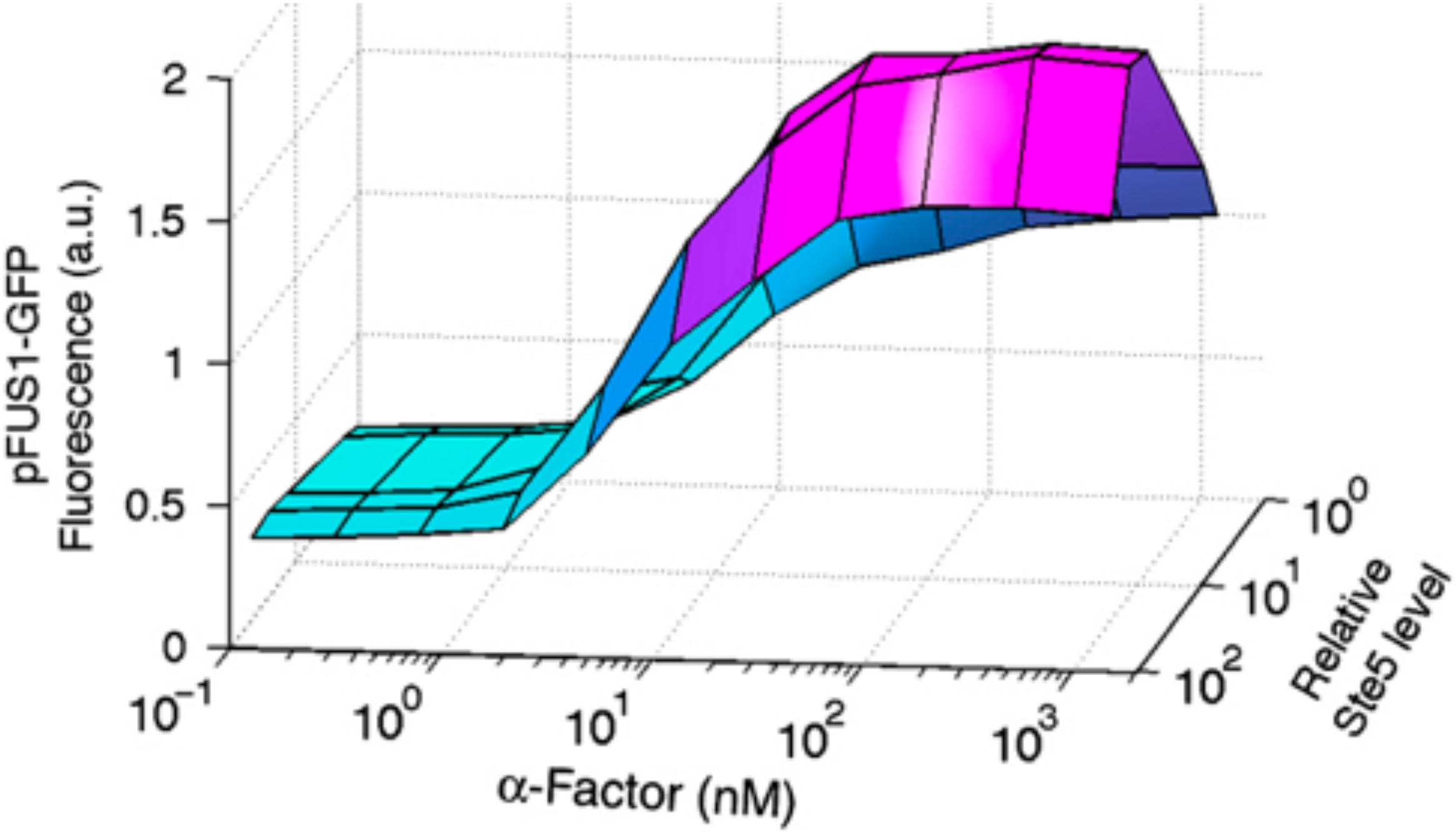


homework! 4

http://www.nature.com/msb/journal/v5/n1/full/msb200973.html

look up fig2 in the above Ref
any relation with our ABC model?

here is (a part of fig2)



homework!

voter model

```
# total population size
%var: 'N' 1000
%var: 'phi_zero' 0.3

# determining the initial minority/majority
%var: 'A0' 'phi_zero' * 'N'
%var: 'A1' (1 - 'phi_zero') * 'N'
```

```
# initial population
%init: 'A0' (A(s~0,a1,a2,a3))
%init: 'A1' (A(s~1,a1,a2,a3))
```

```
# binding rates
%var: 'b' 10
%var: 'bs' 'b'/2

# flipping rates
%var: 'f01' 1
%var: 'f01s' 'f01'/2

%var: 'f10' 1
%var: 'f10s' 'f10'/2

# rewiring rates
%var: 'r0' 1/'N'
%var: 'r0s' 'r0'/2
%var: 'r1' 1/'N'
%var: 'r1s' 'r1'/2
```

```
# 9 binding rules to create the initial graph
# Q1 why the distinction between b and bs?
'bind-11' A(a1),A(a1) -> A(a1!1),A(a1!1)@'bs'
'bind-12' A(a1),A(a2) -> A(a1!1),A(a2!1)@'b'
'bind-13' A(a1),A(a3) -> A(a1!1),A(a3!1)@'b'

'bind-21' A(a2),A(a1) -> A(a2!1),A(a1!1)@'b'
'bind-22' A(a2),A(a2) -> A(a2!1),A(a2!1)@'bs'
'bind-23' A(a2),A(a3) -> A(a2!1),A(a3!1)@'b'

'bind-31' A(a3),A(a1) -> A(a3!1),A(a1!1)@'b'
'bind-32' A(a3),A(a2) -> A(a3!1),A(a2!1)@'b'
'bind-33' A(a3),A(a3) -> A(a3!1),A(a3!1)@'bs'
```

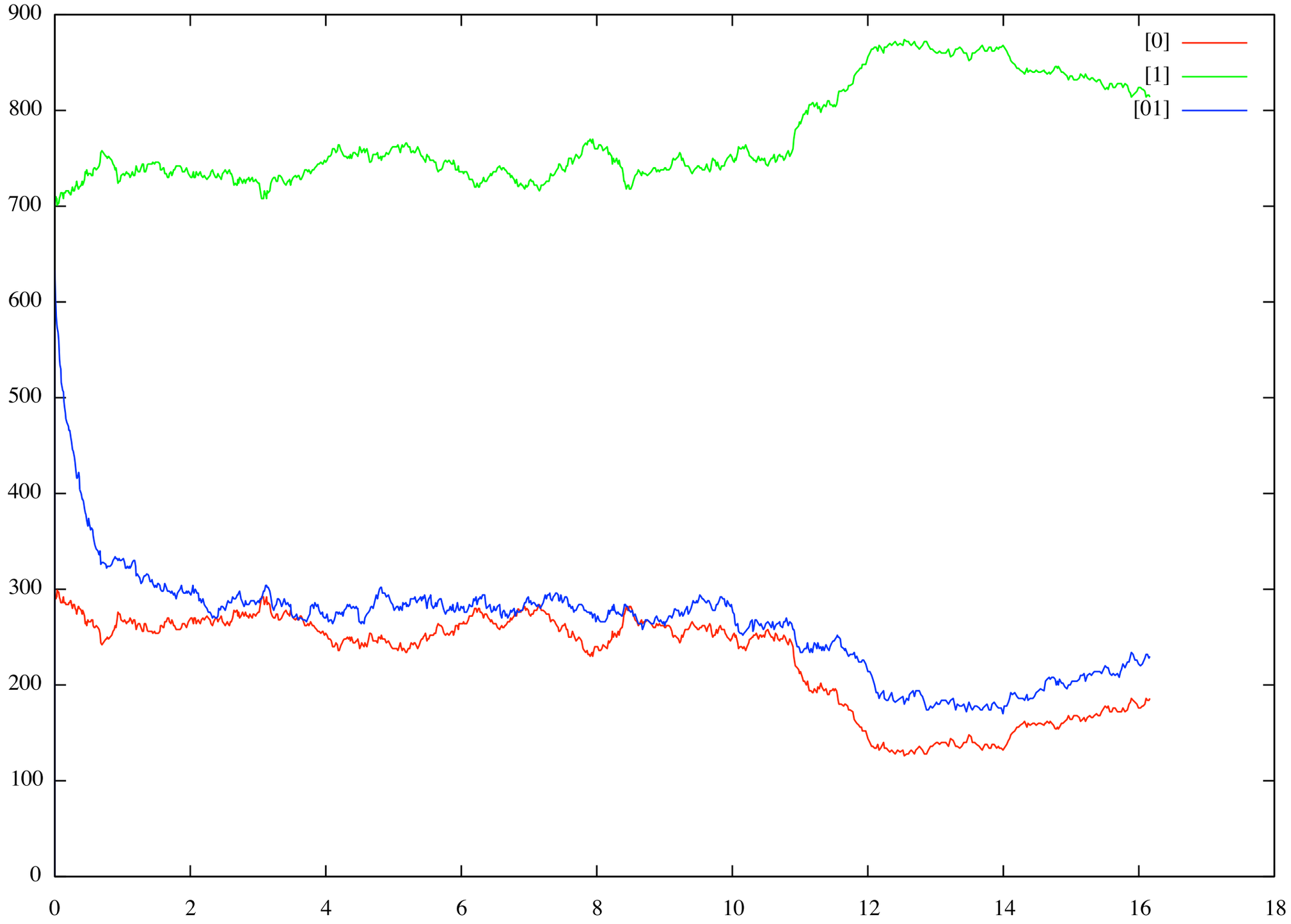
```
# 18 flipping rules
'flip-0-11' A(s~0,a1!1),A(s~1,a1!1) -> A(s~1,a1!1),A(s~1,a1!1)@'f01s'
'flip-0-12' A(s~0,a1!1),A(s~1,a2!1) -> A(s~1,a1!1),A(s~1,a2!1)@'f01'
'flip-0-13' A(s~0,a1!1),A(s~1,a3!1) -> A(s~1,a1!1),A(s~1,a3!1)@'f01'
'flip-0-21' A(s~0,a2!1),A(s~1,a1!1) -> A(s~1,a2!1),A(s~1,a1!1)@'f01'
'flip-0-22' A(s~0,a2!1),A(s~1,a2!1) -> A(s~1,a2!1),A(s~1,a2!1)@'f01s'
'flip-0-23' A(s~0,a2!1),A(s~1,a3!1) -> A(s~1,a2!1),A(s~1,a3!1)@'f01'
'flip-0-31' A(s~0,a3!1),A(s~1,a1!1) -> A(s~1,a3!1),A(s~1,a1!1)@'f01'
'flip-0-32' A(s~0,a3!1),A(s~1,a2!1) -> A(s~1,a3!1),A(s~1,a2!1)@'f01'
'flip-0-33' A(s~0,a3!1),A(s~1,a3!1) -> A(s~1,a3!1),A(s~1,a3!1)@'f01s'

'flip-1-11' A(s~0,a1!1),A(s~1,a1!1) -> A(s~0,a1!1),A(s~0,a1!1)@'f10s'
'flip-1-12' A(s~0,a1!1),A(s~1,a2!1) -> A(s~0,a1!1),A(s~0,a2!1)@'f10'
'flip-1-13' A(s~0,a1!1),A(s~1,a3!1) -> A(s~0,a1!1),A(s~0,a3!1)@'f10'
'flip-1-21' A(s~0,a2!1),A(s~1,a1!1) -> A(s~0,a2!1),A(s~0,a1!1)@'f10'
'flip-1-22' A(s~0,a2!1),A(s~1,a2!1) -> A(s~0,a2!1),A(s~0,a2!1)@'f10s'
'flip-1-23' A(s~0,a2!1),A(s~1,a3!1) -> A(s~0,a2!1),A(s~0,a3!1)@'f10'
'flip-1-31' A(s~0,a3!1),A(s~1,a1!1) -> A(s~0,a3!1),A(s~0,a1!1)@'f10'
'flip-1-32' A(s~0,a3!1),A(s~1,a2!1) -> A(s~0,a3!1),A(s~0,a2!1)@'f10'
'flip-1-33' A(s~0,a3!1),A(s~1,a3!1) -> A(s~0,a3!1),A(s~0,a3!1)@'f10s'
```

```
'rewi-0-223' A(s~0,a2!1),A(s~1,a2!1),A(a3) -> A(s~0,a2!1),A(s~1,a2  ),A(a3!1) @'r0'
'rewi-0-231' A(s~0,a2!1),A(s~1,a3!1),A(a1) -> A(s~0,a2!1),A(s~1,a3  ),A(a1!1) @'r0'
'rewi-0-232' A(s~0,a2!1),A(s~1,a3!1),A(a2) -> A(s~0,a2!1),A(s~1,a3  ),A(a2!1) @'r0'
'rewi-0-233' A(s~0,a2!1),A(s~1,a3!1),A(a3) -> A(s~0,a2!1),A(s~1,a3  ),A(a3!1) @'r0'

'rewi-0-311' A(s~0,a3!1),A(s~1,a1!1),A(a1) -> A(s~0,a3!1),A(s~1,a1  ),A(a1!1) @'r0'
'rewi-0-312' A(s~0,a3!1),A(s~1,a1!1),A(a2) -> A(s~0,a3!1),A(s~1,a1  ),A(a2!1) @'r0'
'rewi-0-313' A(s~0,a3!1),A(s~1,a1!1),A(a3) -> A(s~0,a3!1),A(s~1,a1  ),A(a3!1) @'r0'
'rewi-0-321' A(s~0,a3!1),A(s~1,a2!1),A(a1) -> A(s~0,a3!1),A(s~1,a2  ),A(a1!1) @'r0'
'rewi-0-322' A(s~0,a3!1),A(s~1,a2!1),A(a2) -> A(s~0,a3!1),A(s~1,a2  ),A(a2!1) @'r0'
'rewi-0-323' A(s~0,a3!1),A(s~1,a2!1),A(a3) -> A(s~0,a3!1),A(s~1,a2  ),A(a3!1) @'r0'
'rewi-0-331' A(s~0,a3!1),A(s~1,a3!1),A(a1) -> A(s~0,a3!1),A(s~1,a3  ),A(a1!1) @'r0'
'rewi-0-332' A(s~0,a3!1),A(s~1,a3!1),A(a2) -> A(s~0,a3!1),A(s~1,a3  ),A(a2!1) @'r0'
'rewi-0-333' A(s~0,a3!1),A(s~1,a3!1),A(a3) -> A(s~0,a3!1),A(s~1,a3  ),A(a3!1) @'r0'
```

```
'rewi-1-111' A(s~0,a1!1),A(s~1,a1!1),A(a1) -> A(s~0,a1  ),A(s~1,a1!1),A(a1!1) @'r1'
'rewi-1-112' A(s~0,a1!1),A(s~1,a1!1),A(a2) -> A(s~0,a1  ),A(s~1,a1!1),A(a2!1) @'r1'
'rewi-1-113' A(s~0,a1!1),A(s~1,a1!1),A(a3) -> A(s~0,a1  ),A(s~1,a1!1),A(a3!1) @'r1'
'rewi-1-121' A(s~0,a1!1),A(s~1,a2!1),A(a1) -> A(s~0,a1  ),A(s~1,a2!1),A(a1!1) @'r1'
'rewi-1-122' A(s~0,a1!1),A(s~1,a2!1),A(a2) -> A(s~0,a1  ),A(s~1,a2!1),A(a2!1) @'r1'
'rewi-1-123' A(s~0,a1!1),A(s~1,a2!1),A(a3) -> A(s~0,a1  ),A(s~1,a2!1),A(a3!1) @'r1'
'rewi-1-131' A(s~0,a1!1),A(s~1,a3!1),A(a1) -> A(s~0,a1  ),A(s~1,a3!1),A(a1!1) @'r1'
'rewi-1-132' A(s~0,a1!1),A(s~1,a3!1),A(a2) -> A(s~0,a1  ),A(s~1,a3!1),A(a2!1) @'r1'
'rewi-1-133' A(s~0,a1!1),A(s~1,a3!1),A(a3) -> A(s~0,a1  ),A(s~1,a3!1),A(a3!1) @'r1'

'rewi-1-211' A(s~0,a2!1),A(s~1,a1!1),A(a1) -> A(s~0,a2  ),A(s~1,a1!1),A(a1!1) @'r1'
'rewi-1-212' A(s~0,a2!1),A(s~1,a1!1),A(a2) -> A(s~0,a2  ),A(s~1,a1!1),A(a2!1) @'r1'
'rewi-1-213' A(s~0,a2!1),A(s~1,a1!1),A(a3) -> A(s~0,a2  ),A(s~1,a1!1),A(a3!1) @'r1'
'rewi-1-221' A(s~0,a2!1),A(s~1,a2!1),A(a1) -> A(s~0,a2  ),A(s~1,a2!1),A(a1!1) @'r1'
```

```
%var: '[0]' A(s~0)
%var: '[1]' A(s~1)

%var: '01-11' A(s~0,a1!1),A(s~1,a1!1)
%var: '01-12' A(s~0,a1!1),A(s~1,a2!1)
%var: '01-13' A(s~0,a1!1),A(s~1,a3!1)
%var: '01-21' A(s~0,a2!1),A(s~1,a1!1)
%var: '01-22' A(s~0,a2!1),A(s~1,a2!1)
%var: '01-23' A(s~0,a2!1),A(s~1,a3!1)
%var: '01-31' A(s~0,a3!1),A(s~1,a1!1)
%var: '01-32' A(s~0,a3!1),A(s~1,a2!1)
%var: '01-33' A(s~0,a3!1),A(s~1,a3!1)

%var: '[01]' '01-11' + '01-12' + '01-13' + \
             '01-21' + '01-22' + '01-23' + \
             '01-31' + '01-32' + '01-33'
```

```
%plot: '[0]'
%plot: '[1]'
%plot: '[01]'

%def: "dumpInfluenceMap" "no"
%def: "dotSnapshots" "yes"

%mod: [E]>10000 do $SNAPSHOT
```



Sunday, 30 November 14