# Simulations

These scripts are for the SPiM Player stochastic  $\pi$ -calculus simulator v1.13 [15], and Matlab 7.4.0 (ode45). The core SPiM syntax maps directly to stochastic  $\pi$ -calculus [17,18]. The SPiM scripts are complete and executable, and usually are a literal translation of the automata in the figures, with some additional code for plotting directives and for test signals. Figure 2 and Figure 36 instead outline the encoding of automata used in the other scripts.

## **Figure 2: Automata reactions**

SPiM encoding of Delay at rate r from state A to state B, then running 100 automata with initial state A:

```
let A() = delay@r; B() and B() = ... run 100 of A()
```

Encoding of Interaction: an input ?a from state A1 to A2 and an ouput !a from state B1 to B2, over a channel of rate r, between two concurrent automata initially in states A1 and B1.

```
new a@r:chan
let A1() = ?a; A2() and A2() = ...
let B1() = !a; B2() and B2() = ...
run (A1() | B1())
```

SPiM encoding of multiple transitions (a delay, an input, and an output) from the same state A to three different states:

let A() = do delay@r; B1() or ?a; B2() or !b; B3()

## Figure 3: Celebrity automata

directive sample 0.1 directive plot A(); B() new a@1.0:chan new b@1.0:chan let A() = do !a; A() or ?a; B() and B() = do !b; B() or ?b; A() run 100 of (A() | B())

#### Figure 5: Groupie automata

directive sample 2.0
directive plot A(); B()
new a@1.0:chan
new b@1.0:chan
let A() = do !a; A() or ?b; B()
and B() = do !b; B() or ?a; A()
run 100 of (A() | B())

#### **Figure 6: Both together**

directive sample 10.0
directive plot Ag(); Bg(); Ac(); Bc()
new a@1.0:chan
new b@1.0:chan
let Ac() = do !a; Ac() or ?a; Bc()
and Bc() = do !b; Bc() or ?b; Ac()
let Ag() = do !a; Ag() or ?b; Bg()
and Bg() = do !b; Bg() or ?a; Ag()
run 1 of Ac()
run 100 of (Ag() | Bg())

#### **Figure 7: Hysteric groupies**

directive sample 10.0
directive plot A(); B()
new a@1.0:chan
new b@1.0:chan
let A() = do !a; A() or ?b; ?b; ?b; B()
and B() = do !b; B() or ?a; ?a; ?a; A()
let Ad() = !a; Ad()
and Bd() = !b; Bd()

run 100 of (A() | B()) run 1 of (Ad() | Bd())

### **Figure 9: Sequence of delays**

```
directive sample 20.0
directive plot S1(); S2(); S3(); S4(); S5(); S6();
S7(); S8(); S9(); S10()
let S1() = delay@1.0; S2() and S2() = delay@1.0; S3()
and S3() = delay@1.0; S4() and S4() = delay@1.0; S5()
and S5() = delay@1.0; S6() and S6() = delay@1.0; S7()
and S7() = delay@1.0; S8() and S8() = delay@1.0; S9()
and S9() = delay@1.0; S10() and S10() = ()
run 10000 of S1()
```

### Figure 11: All 3 reactions in 1 automaton

```
directive sample 0.02
directive plot A(); B()
new a@1.0:chan
new b@1.0:chan
let A() = do !a; A() or !b; A() or ?b; B()
and B() = do delay@1.0; A() or ?a; A()
run 1000 of B()
```

#### **Figure 12: Same behavior**

directive sample 0.02 directive plot A(); B() new a@1.0:chan new b@0.5:chan let A() = do !a; A() or !b; B() or ?b; B() and B() = do delay@1.0; A() or ?a; A() run 1000 of B()

## **Figure 13: Sequence of interactions**

```
directive sample 0.02
directive plot A1(); A2(); A3(); A4(); A5(); A6();
A7(); A8(); A9(); A10()
new al@1.0:chan new a2@1.0:chan new a3@1.0:chan
new a4@1.0:chan new a5@1.0:chan new a6@1.0:chan
new a7@1.0:chan new a8@1.0:chan new a9@1.0:chan
let A1() = ?a1; A2() and B1() = !a1; B2()
and A2() = ?a2; A3() and B2() = !a2; B3()
and A3() = ?a3; A4() and B3() = !a3; B4()
and A4() = ?a4; A5() and B4() = !a4; B5()
and A5() = ?a5; A6() and B5() =
                                !a5; B6()
and A6() = ?a6; A7() and B6() = !a6; B7()
and A7() = ?a7; A8() and B7() = !a7; B8()
and A8() = ?a8; A9() and B8() = !a8; B9()
and A9() = ?a9; A10() and B9() = !a9; B10()
and A10() = () and B10() = ()
run 5000 of (A1() | B1())
```

#### **Figure 14: Zero order reactions**

directive sample 1000.0
directive plot S(); P(); E()
new a@1.0:chan
let E() = !a; delay@1.0; E()
and S() = ?a; P()
and P() = ()
run (1 of E() | 1000 of S())

#### **Figure 15: Subtraction**

```
directive sample 20.0 1000
directive plot E(); F()
new a@1.0:chan
let E() = ?a; delay@1.0; E()
and F() = !a; delay@1.0; F()
let raising(p:proc(), t:float) =
 (* Produce one p() every t sec with precision dt *)
 (val dt= 100.0 run step(p, t, dt, dt))
and step(p:proc(), t:float, n:float, dt:float) =
 if n<=0.0 then (p()!step(p,t,dt,dt))
 else delay@dt/t; step(p,t,n=1.0,dt)
run 1000 of F()
```

```
run raising(E,0.01)
```

directive sample 20.0 1000
directive plot E(); F()
new a@l.0:chan
let E() = ?a; E()
and F() = !a; F()
let raising(p:proc(), t:float) =

... see code for Error! Reference source not found.
run 1000 of F()
run raising(E,0.01)

## Figure 16: Ultrasensitivity

directive sample 215.0
directive plot E();F();S();P();ES();FP()
new a@1.0:chan new b@1.0:chan
let S() = ?a; P()
and P() = ?b; S()
let E() = !a; ES()
and ES() = delay@1.0; E()
and F() = !b; FP()
and FP() = delay@1.0; F()
run 1000 of S()
let raising(p:proc(), t:float) =
 ... see code for Error! Reference source not found.
run 100 of F()
run raising(E,1.0)

## Figure 17: Positive feedback transition

directive sample 0.02 1000 directive plot B(); A() val s=1.0 new b@s:chan let A() = ?b; B() and B() = !b;B() run (1000 of A() | 1 of B())

## Figure 18: Bell shape

directive sample 0.003 1000
directive plot B(); A(); C()
new b@1.0:chan new c@1.0:chan
let A() = ?b; B()
and B() = do !b;B() or ?c; C()
and C() = !c;C()
run ((10000 of A()) | B() | C())

## Figure 19: Oscillator

directive sample 0.03 1000 directive plot A(); B(); C() new a@1.0:chan new b@1.0:chan new c@1.0:chan let A() = do !a;A() or ?b; B() and B() = do !b;B() or ?c; C() and C() = do !c;C() or ?a; A() run (900 of A() | 500 of B() | 100 of C())

## Figure 20: Positive two-stage feedback

```
directive sample 0.1 1000
directive plot B(); A(); A1()
val s=1.0
new c@s:chan
let A() = ?c; A1()
and A1() = ?c; B()
and B() = !c;B()
run (1000 of A() | 1 of B())
```

## Figure 21: Square shape

directive sample 0.2 1000 directive plot B(); A(); A1(); B1(); C() new b@1.0:chan new c@1.0:chan let A() = ?b; A1() and A1() = ?b; B() and B() = do !b;B() or ?c; B1()
and B1() = ?c; C()
and C() = !c;C()
run ((1000 of A()) | B() | C())

## Figure 22: Hysteric 3-way groupies

directive sample 0.5 1000
directive plot A(); B(); C()
new a@1.0:chan
new b@1.0:chan
new c@1.0:chan
let A() = do !a; A() or ?c; ?c; C()
and B() = do !b; B() or ?a; ?a; A()
and C() = do !c; C() or ?b; ?b; B()
let Ad() = !a; Ad()
and Bd() = !b; Bd()
and Cd() = !c; Cd()
run 1000 of A()
run 1 of (Ad() | Bd() | Cd())

## Figure 23: Second-order cascade

directive sample 0.03 directive plot !a; !b; !c new a@1.0:chan new b@1.0:chan new c@1.0:chan let Amp\_hi(a:chan, b:chan) = do !b; Amp\_hi(a,b) or delay@1.0; Amp\_lo(a,b) and Amp\_lo(a:chan, b:chan) = ?a; Amp\_hi(a,b) run 1000 of (Amp\_lo(a,b) | Amp\_lo(b,c)) let A() = !a; A() run 100 of A()

## Figure 24: Zero-order cascade

directive sample 0.01 directive plot !a; !b; !c new a@1.0:chan new b@1.0:chan new c@1.0:chan let Amp\_hi(a:chan, b:chan) = do !b; delay@1.0; Amp\_hi(a,b) or delay@1.0; Amp\_lo(a,b) and Amp\_lo(a:chan, b:chan) = ?a; Amp\_hi(a,b) run 1000 of (Amp\_lo(a,b) | Amp\_lo(b,c)) let A() = !a; delay@1.0; A() run 100 of A() directive sample 20.0

directive plot !a; !b; !c
new a@1.0:chan new b@1.0:chan new c@1.0:chan
let Amp\_hi(a:chan, b:chan) =
 do !b; delay@1.0; Amp\_hi(a,b)
 or delay@1.0; Amp\_lo(a,b)
and Amp\_lo(a:chan, b:chan) =
 ?a; Amp\_hi(a,b)
run 1000 of (Amp\_lo(a,b) | Amp\_lo(b,c))
let A() = !a; delay@1.0; A()
run 100 of A()
Figure 25: Zero-order transduction

directive sample 10.0
directive plot !a; !b
new a@1.0:chan new b@1.0:chan
let Amp\_hi(a:chan, b:chan) =
 do !b; delay@1.0; Amp\_hi(a,b)
 or delay@1.0; Amp\_lo(a,b)
and Amp\_lo(a:chan, b:chan) =
 ?a; Amp\_hi(a,b)
run 1000 of Amp\_lo(a,b)

let A() = !a; delay@1.0; A()
run 900 of A()

## Figure 26: Second-order double cascade

directive sample 0.03 directive plot !a; !b; !c

```
new a@1.0:chan new b@1.0:chan new c@1.0:chan
let Amp hi(a:chan, b:chan) =
 do !b; Amp_hi(a,b) or delay@1.0; Amp_lo(a,b)
and Amp_lo(a:chan, b:chan) =
 ?a; ?a; Amp hi(a,b)
run 1000 of (Amp lo(a,b) | Amp lo(b,c))
let A() = !a; A()
run 100 of A()
```

## Figure 27: Zero-order double cascade

```
directive sample 0.03
directive plot !a; !b
new a@1.0:chan new b@1.0:chan
let Amp_hi(a:chan, b:chan)
  do !b; delay@1.0; Amp_hi(a,b)
  or delay@1.0; Amp_lo(a,b)
and Amp_lo(a:chan, b:chan) =
 ?a; ?a; Amp_hi(a,b)
run 1000 of Amp lo(a,b)
let A() = !a; delay@1.0; A()
run 2000 of A()
```

#### **Figure 28: Simple inverter**

```
directive sample 110.0 1000
 directive plot !a; !b; !c
 new a@1.0:chan new b@1.0:chan new c@1.0:chan
 let Inv hi(a:chan, b:chan) =
      do !b; Inv_hi(a,b)
or ?a; Inv_lo(a,b)
 and Inv lo(a:chan, b:chan) =
      delay@1.0; Inv hi(a,b)
 run 100 of (Inv_hi(a,b) | Inv_lo(b,c))
run 100 of (Inv_n1(a,b) | Inv_lo(b,C))
let clock(t:float, tick:chan) =
  (val dt=100.0 run step(tick, t, dt, dt))
and step(tick:chan, t:float, n:float, dt:float) =
  if n<=0.0 then !tick; clock(t,tick)
  else delay@dt/t; step(tick,t,n-1.0,dt)
let S1(a:chan, tock:chan) =
  do !a; S1(a,tock) or ?tock; ()
and SN(n:int, t:float, a:chan, tick:chan, tock:chan) =
  if n=0 then clock(t, tock)
  else ?tick; (S1(a,tock) | SN(n-1,t,a,tick,tock))
let raisingfalling(a:chan, n:int, t:float) =
  (new tick:chan new tock:chan
  run (clock(t,tick) | SN(n,t,a,tick,tock)))</pre>
```

run raisingfalling(a,100,0.5)

directive sample 15.0 1000 directive plot !a; !b; !c; !d; !e; !f new a@1.0:chan new b@1.0:chan new c@1.0:chan new d@1.0:chan new e@1.0:chan new f@1.0:chan let Inv\_hi(a:chan, b:chan) = do !b; Inv\_hi(a,b)
or ?a; Inv\_lo(a,b) and Inv lo(a:chan, b:chan) = delay@1.0; Inv\_hi(a,b) run 100 of (Inv\_lo(a,b) | Inv\_lo(b,c)
| Inv\_lo(c,d) | Inv\_lo(d,e) | Inv\_lo(e,f))

directive sample 2.0 1000 directive plot !a; !b; !c new a@1.0:chan new b@1.0:chan new c@1.0:chan let Inv hi(a:chan, b:chan) = do !b; Inv\_hi(a,b)
or ?a; Inv\_lo(a,b) and Inv\_lo(a:chan, b:chan) =
 delay@1.0; Inv\_hi(a,b) run 100 of (Inv\_hi(a,b) | Inv\_lo(b,c) | Inv\_lo(c,a))

#### **Figure 29: Feedback inverter**

directive sample 110.0 1000 directive plot !a; !b; !c new a@1.0:chan new b@1.0:chan new c@1.0:chan let Inv\_hi(a:chan, b:chan) = do !b; Inv\_hi(a,b) or ?a; Inv\_lo(a,b) and Inv\_lo(a:chan, b:chan) =
 do delay@1.0; Inv\_hi(a,b) or ?b; Inv\_hi(a,b) run 100 of (Inv hi(a,b) | Inv lo(b,c))

let raisingfalling(a:chan, n:int, t:float) =
 ... see code for Error! Reference source not found. run raisingfalling(a,100,0.5)

directive sample 1.0 1000 directive plot !a; !b; !c; !d; !e; !f new a@1.0:chan new b@1.0:chan new c@1.0:chan new d@1.0:chan new e@1.0:chan new f@1.0:chan let Inv\_hi ... and Inv\_lo ...
... see code above

run 100 of (Inv\_lo(a,b) | Inv\_lo(b,c)
| Inv\_lo(c,d) | Inv\_lo(d,e) | Inv\_lo(e,f))

```
directive sample 2.0 1000
directive plot !a; !b; !c
```

new a@1.0:chan new b@1.0:chan new c@1.0:chan

let Inv\_hi ... and Inv\_lo ... ... see code above

run 100 of (Inv hi(a,b) | Inv lo(b,c) | Inv lo(c,a))

## **Figure 30: Double-height inverter**

```
directive sample 110.0 1000
directive plot !a; !b; !c
new a@1.0:chan new b@1.0:chan new c@1.0:chan
let Inv2_hi(a:chan, b:chan) =
do !b; Inv2_hi(a,b) or ?a; Inv2_mi(a,b)
and Inv2_mi(a:chan, b:chan) =
 do delay@1.0; Inv2_hi(a,b)
or ?a; Inv2_lo(a,b)
and Inv2_lo(a:chan, b:chan) =
 delay@1.0; Inv2_mi(a,b)
run 100 of (Inv2_hi(a,b) | Inv2_lo(b,c))
let raisingfalling(a:chan, n:int, t:float) =
    ... see code for Error! Reference source not found.
run raisingfalling(a,100,0.5)
directive sample 15.0 1000
directive plot !a; !b; !c; !d; !e; !f
new a@1.0:chan new b@1.0:chan new c@1.0:chan
new d@1.0:chan new e@1.0:chan new f@1.0:chan
let Inv2_hi ... and Inv2_lo ...
   ... see code above
```

run 100 of (Inv2\_lo(a,b) | Inv2\_lo(b,c)
| Inv2\_lo(c,d) | Inv2\_lo(d,e) | Inv2\_lo(e,f))

directive sample 2.0 1000 directive plot !a; !b; !c

new a@1.0:chan new b@1.0:chan new c@1.0:chan let Inv2\_hi ... and Inv2\_lo ... ... see code above run 100 of (Inv2 hi(a,b) | Inv2 lo(b,c) | Inv2 lo(c,a))

## Figure 31: Double-height feedback inverter

```
directive sample 110.0 1000
directive plot !a; !b; !c
new a@1.0:chan new b@1.0:chan new c@1.0:chan
let Inv2_hi(a:chan, b:chan)
  do !b; Inv2_hi(a,b) or ?a; Inv2_mi(a,b)
and Inv2_mi(a:chan, b:chan) =
    do delay@1.0; Inv2_hi(a,b)
    or ?a; Inv2_lo(a,b)
    or ?b; Inv2_hi(a,b)
and Inv2_lo(a:chan, b:chan) =
  do delay@1.0; Inv2 mi(a,b)
  or ?b; Inv2_mi(a,b)
run 100 of (Inv2_hi(a,b) | Inv2_lo(b,c))
let raisingfalling(a:chan, n:int, t:float) =
  ... see code for Error! Reference source not found.
run raisingfalling(a,100,0.5)
directive sample 1.0 1000
directive plot !a; !b; !c; !d; !e; !f
```

```
new a@1.0:chan new b@1.0:chan new c@1.0:chan
new d@1.0:chan new e@1.0:chan new f@1.0:chan
let Inv2_hi ... and Inv2_lo ...
   ... see code above
```

run 100 of (Inv2\_lo(a,b) | Inv2\_lo(b,c)
| Inv2\_lo(c,d) | Inv2\_lo(d,e) | Inv2\_lo(e,f))

directive sample 2.0 1000 directive plot !a; !b; !c

new a@1.0:chan new b@1.0:chan new c@1.0:chan
let Inv2\_hi ... and Inv2\_lo ...

## Figure 32: Or and And

directive sample 10.0 1000 directive plot !a; !b; !c new a@1.0:chan new b@1.0:chan new c@1.0:chan val del = 1.0 let Or hi(a:chan, b:chan, c:chan) = do !c; Or\_hi(a,b,c) or delay@del; Or\_lo(a,b,c) and Or\_lo(a:chan, b:chan, c:chan) = do ?a; Or\_hi(a,b,c) or ?b; Or\_hi(a,b,c) run 1000 of Or\_lo(a,b,c) let clock(t:float, tick:chan) = (val dt=100.0 run step(tick, t, dt, dt)) and step(tick:chan, t:float, n:float, dt:float) =
 if n<=0.0 then !tick; clock(t,tick)</pre> else delay@dt/t; step(tick,t,n-1.0,dt) let S\_a(tick:chan) = do !a; S\_a(tick) or ?tick; ()
let S\_b(tick:chan) = ?tick; S\_b1(tick) and S\_b1(tick:chan) = do !b; S b1(tick) or ?tick; S b2(tick) and S b2(tick:chan) = do !b; S  $\overline{b2}$ (tick) or ?tick; () let many(n:float, p:proc(float), nt:float) = if  $n\leq=0.0$  then () else (p(nt) | many(n-1.0, p, nt))

let BoolInputs(n:float, nt:float, m:float, mt:float) =
(run many(n, Sig\_a, nt) run many(m, Sig\_b, mt))
and Sig\_a(nt:float) =
 (new tick:chan run (clock(nt,tick) | S\_a(tick)))
and Sig\_b(mt:float) =

(new tick:chan run (clock(mt,tick) | S\_b(tick)))
run BoolInputs(100.0, 4.0, 100.0, 2.0)

directive sample 10.0 1000
directive plot !a; !b; !c
new a@l.0:chan new b@l.0:chan new c@l.0:chan
val del = 1.0
let And\_hi(a:chan, b:chan, c:chan) =
 do !c; And\_hi(a,b,c) or delay@del; And\_lo\_a(a,b,c)
and And\_lo\_a(a:chan, b:chan, c:chan) =
 do ?a; And\_hi(a,b,c) or delay@del; And\_lo\_b(a,b,c)
and And\_lo\_b(a:chan, b:chan, c:chan) =
 ?b; And\_lo\_a(a,b,c)
run 1000 of And\_lo\_b(a,b,c)
let BoolInputs(n:float, nt:float, m:float, mt:float) =
 ... see code for Error! Reference source not found.

run BoolInputs(100.0, 4.0, 100.0, 2.0)

## Figure 33: Imply and Xor

directive sample 15.0 1000 directive plot !a; !b; !c new a@1.0:chan new b@1.0:chan new c@1.0:chan val del = 1.0 let Imply\_hi\_a(a:chan, b:chan, c:chan) = do !c; Imply\_hi\_a(a,b,c) or ?a; Imply\_lo(a,b,c) and Imply\_hi\_b(a:chan, b:chan, c:chan) = do !c; Imply\_hi\_b(a,b,c) or delay@del; Imply\_lo(a,b,c) and Imply\_lo(a:chan, b:chan, c:chan) = do ?b; Imply\_hi\_b(a,b,c) or delay@del; Imply\_hi\_a(a,b,c) run 1000 of Imply\_lo(a,b,c) let BoolInputs(n:float, nt:float, m:float, mt:float) = ... see code for Error! Reference source not found.

run BoolInputs(100.0, 4.0, 100.0, 2.0)

directive sample 20.0 1000 directive plot !a; !b; !c

new a@1.0:chan new b@1.0:chan new c@1.0:chan let Xor\_hi\_a(a:chan, b:chan, c:chan) = do !c; Xor\_hi\_a(a,b,c) or ?b; Xor\_lo\_ab(a,b,c) or delay@1.0; Xor\_lo\_a(a,b,c) and Xor\_hi\_b(a:chan, b:chan, c:chan) = do !c; Xor\_hi\_b(a,b,c) or ?a; Xor\_lo\_ab(a,b,c) or delay@1.0; Xor\_lo\_b(a,b,c) and Xor lo a(a:chan, b:chan, c:chan) = do ?a; Xor\_hi\_a(a,b,c) or ?b; Xor\_lo\_ab(a,b,c) and Xor\_lo\_b(a:chan, b:chan, c:chan) =
 do ?b; Xor\_hi\_b(a,b,c) or ?a; Xor\_lo\_ab(a,b,c) and Xor lo ab(a:chan, b:chan, c:chan) do delay@1.0; Xor\_hi\_a(a,b,c) or delay@1.0; Xor\_hi\_b(a,b,c) run 500 of (Xor lo a(a,b,c) | Xor\_lo\_b(a,b,c)) let BoolInputs(n:float, nt:float, m:float, mt:float) = ... see code for Error! Reference source not found. run BoolInputs(100.0, 8.0, 100.0, 4.0) **Figure 34: Memory Elements** (\* Top Left, Top Center \*) directive sample 0.1 directive plot A(); B(); C() new a@1.0:chan new b@1.0:chan let A() = do !a; A() or ?b; C() and C() = do ?a; A() or ?b; B() and B() = do !b; B() or ?a; C() run 100 of (A() | B()) (\* Bottom Left \*) directive sample 1.0 directive plot A(); B(); C() new a@1.0:chan new b@1.0:chan let A() = do !a; A() or ?b; C() and C() = do ?a; A() or ?b; B() and B() = do !b; B() or ?a; C()let Ad() = !a; Ad()and Bd() = !b; Bd()run 100 of (A() | B()) run 10 of (Ad() | Bd()) (\* Bottom Center \*) directive sample 0.6 directive plot A(); B(); C() new a@1.0:chan new b@1.0:chan

let A() = do !a; A() or ?b; C() and C() = do ?a; A() or ?b; B() and B() = do !b; B() or ?a; C() let Ad() = !a; Ad() run 100 of (A() | B()) run 100 of delay@10.0; delay@10.0; delay@10.0; delay@10.0; Ad()

#### Figure 35: Discrete vs. Continuous Modeling

(* Top Left *) (A) dx1/dt = -(x1-x2) (B) dx2/dt = (x1-x2)	initially x1 = 2000.0 x2 = 0.0
(* Top Center *) (A) dx1/dt=x1*x4-x3*x1-x1+x4 (A') dx2/dt=x3*x1-x3*x2+x1-x2 (B) dx3/dt=x3*x2-x1*x3-x3+x2 (B') dx4/dt=x1*x3-x1*x4+x3-x4	initially x1 = 2000.0 x2 = 0.0 x3 = 0.0 x4 = 0.0
<pre>(* Top Right *) (A) dx1/dt=x1*x6-x3*x1-x1+x6 (A') dx2/dt=x3*x1-x3*x2+x1-x2 (A") dx5/dt=x3*x2-x3*x5+x2-x5 (B) dx3/dt=x3*x5-x1*x3-x3+x5 (B') dx4/dt=x1*x3-x1*x4+x3-x4 (B") dx6/dt=x1*x4-x1*x6+x4-x6</pre>	initially x1 = 2000.0 x2 = 0.0 x5 = 0.0 x3 = 0.0 x4 = 0.0 x6 = 0.0
(* Bottom Left *) directive sample 5.0 1000 directive plot B(); A()	
new a@1.0:chan new b@1.0:chan	

let A() = do !a; A() or ?b; B()

and B() = do !b; B() or ?a; A()
let Ad() = !a; Ad()

and Bd() = !b; Bd() run 2000 of A() run 1 of (Ad() | Bd())

(\* Bottom Center \*)
Same as Bottom Left, except:
let A() = do !a; A() or ?b; ?b; B()
and B() = do !b; B() or ?a; ?a; A()
(\* Bottom Right \*)
Center Bottem Left

Same as Bottom Left, except: let A() = do !a; A() or ?b; ?b; ?b; B() and B() = do !b; B() or ?a; ?a; ?a; A()

## **Figure 36: Polyautomata reactions**

SPiM encoding of Association over channel  $a@r_0/r_1$  of arity 1, with one automaton performing an output from state A to A1 and the other automaton performing an input from state B to B1:

new a@r0:chan(chan)
let A() = (new kl@r1:chan run !a(k1); A1(k1))
and B() = ?a(k1); B1(k1)

Encoding of Dissociation through the previously shared k1.

and A1(k1:chan) = !k1; A() and B1(k1:chan) = ?k1; B()

More generally, for a@ $r_0$ ,..., $r_{n-1}$  we declare an (n-1)-ary channel:

new a@r<sub>0</sub>:chan(chan,...,chan) (\*n-1 times\*)

Association then creates n-1 shared dissociation channels:

and then A1 can choose which channel to use for dissociation. Note that the constraint about not reassociating before a dissociation is not automatically enforced by this encoding.

#### Figure 37: Complexation/decomplexation

directive sample 0.005 directive plot !A\_f; !A\_b; !B\_f; !B\_b new A\_f:chan new A\_b:chan new B\_f:chan new B\_b:chan val mu = 1.0 val lam = 1.0 new a@mu:chan(chan) let Af() = (new k@lam:chan run do !a(k); Ab(k) or !A\_f) and Ab(k:chan) = do !k; Af() or !A\_b let Bf() = do ?a(k); Bb(k) or !B\_f and Bb(k:chan) = do ?k; Bf() or !B\_b run (1000 of Af() | 500 of Bf())

#### **Figure 38: Enzymatic reactions**

```
directive sample 0.05 1000
directive plot !E_f; !E_b; !S_f; !S_b; !P_
new E_f:chan new E_b:chan
new S_f:chan new S_b:chan new P_:chan
val r0 = 1.0 val r1 = 1.0 val r2 = 100.0
new a@r0:chan(chan,chan)
let P() = !P_
let Ef() =
    (new kl@r1:chan new k2@r2:chan
    run do !a(k1,k2); Eb(k1,k2) or !E_f)
and Eb(k1:chan,k2:chan) =
    do !k1; Ef() or !k2; Ef() or !E_b
let Sf() = do ?a(k1,k2); Sb(k1,k2) or !S_f
and Sb(k1:chan,k2:chan) =
    do ?k1; Sf() or ?k2; P() or !S_b
run (1000 of Ef() | 2000 of Sf())
```

## **Figure 39: Homodimerization**

```
directive sample 0.005 10000
directive plot !A_f; !A_i; !A_o
new A_f:chan new A_i:chan new A_o:chan
new a@1.0:chan(chan)
```

let Af() =

(new k@1.0:chan run do ?a(k); Ai(k) or !a(k); Ao(k) or !A\_f) and Ai(k:chan) = do ?k; Af() or !A\_i and Ao(k:chan) = do !k; Af() or !A\_o run 1000 of Af()

## Figure 40: Bidirectional polymerization

directive sample 1000.0 directive plot ?count type Link = chan(chan) type Barb = chan val lam = 1000.0 (\* set high for better counting \*) val mu = 1.0 new c@mu:chan(Link) new enter@lam:chan(Barb) new count@lam:Barb let Af() = (new rht@lam:Link run do !c(rht); Ar(rht) or ?c(lft); Al(lft)) and Al(lft:Link) = (new rht@lam:Link run !c(rht); Ab(lft,rht)) and Ar(rht:Link) = ?c(lft); Ab(lft,rht) and Ab(lft:Link, rht:Link) = do ?enter(barb); (?barb | !rht(barb)) or ?lft(barb); (?barb | !rht(barb)) (\* each Abound waits for a barb, exhibits it, and passes it to the right so we can plot number of Abound in a ring \*) let clock(t:float, tick:chan) =
 (val dt=100.0 run step(tick, t, dt, dt))
and step(tick:chan, t:float, n:float, dt:float) =
 if n<=0.0 then !tick; clock(t,tick) else delay@dt/t;
step(tick,t,n-1.0,dt)</pre> new tick:chan let Scan() = ?tick; !enter(count); Scan() run 1000 of Af() run (clock(100.0, tick) | Scan())

## Figure 42: Actin-like polymerization

```
directive sample 0.01 (* 0.25, 35.0 *) 1000
directive plot !A_f; !A_l; !A_r; !A_b
new A_f:chan new A_l:chan new A_r:chan new A_b:chan
val lam = 1.0 (* dissoc *)
val mu = 1.0 (* assoc *)
new c@mu:chan(chan)
let Af() =
  (new lft@lam:chan run
   do !c(lft); Al(lft)
   or ?c(rht); Ar(rht) or !A f)
and Al(lft:chan) =
   do !lft; Af()
   or ?c(rht); Ab(lft,rht) or !A l
and Ar(rht:chan) =
  do ?rht; Af() or !A r
and Ab(lft:chan, rht:chan) =
   do !lft; Ar(rht) or !A b
run 1000 of Af()
```