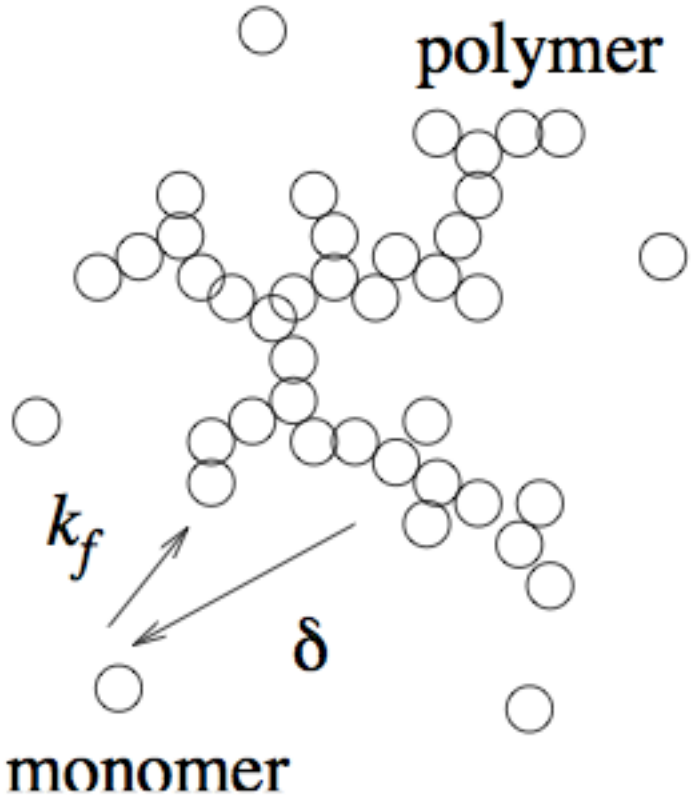
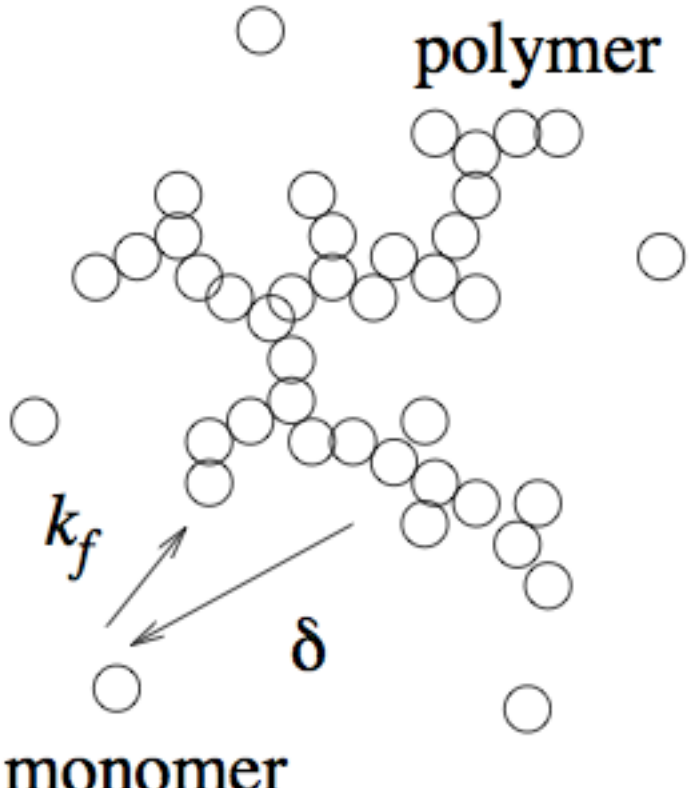
Simple models for polymerization

(1) Aggregation of monomers



Every site on polymer is available for further growth

Definitions



$c(t) =$ number of monomer subunits in the volume at time t,

$F(t) =$ amount of polymer (in number of monomer equivalents) at time t,

$A(t) =$ total amount of material (in number of monomer equivalents) at time t.

Kinetics (mass action)

$c(t) =$ number of monomer subunits in the volume at time t,

$F(t) =$ amount of polymer (in number of monomer equivalents) at time t,

$A(t) =$ total amount of material (in number of monomer equivalents) at time t.

$$\frac{dc}{dt} = -k_f cF + \delta F,$$

$$\frac{dF}{dt} = k_f cF - \delta F.$$

Note: Total amount $A = c + F$ is constant

Simulations

```
dc/dt=-kf*c*F +kr*F
dF/dt=kf*c*F -kr*F
param kf=1, kr=1
init c=0.7, F=0.1
done
```

Simplify (eliminate *F*)

$$\frac{dc}{dt} = (-k_f c + \delta)F = k_f(A - c)\left(\frac{\delta}{k_f} - c\right)$$

Critical concentration

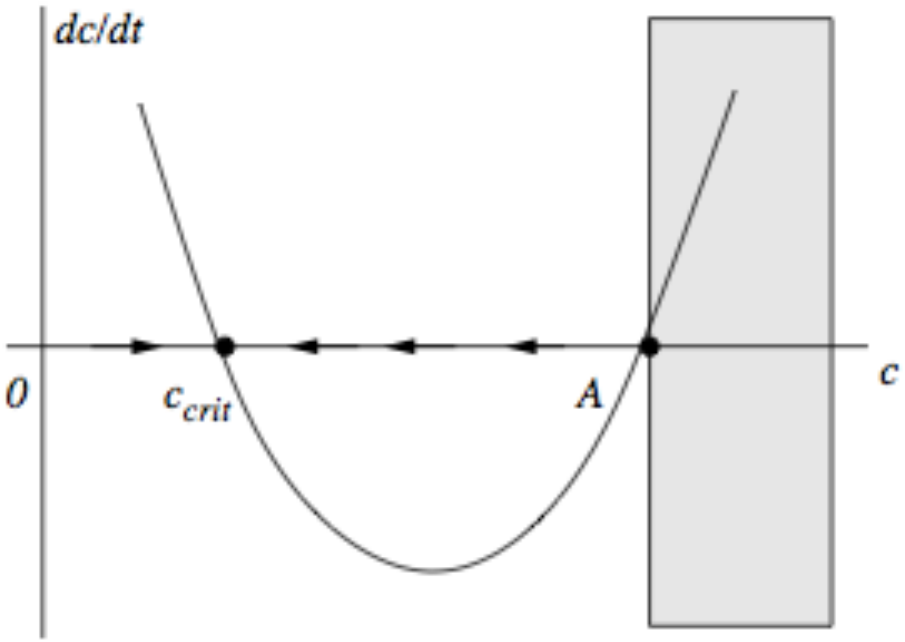
Rewrite as:

$$\frac{dc}{dt} = k_f(A - c)(c_{crit} - c).$$

Predictions

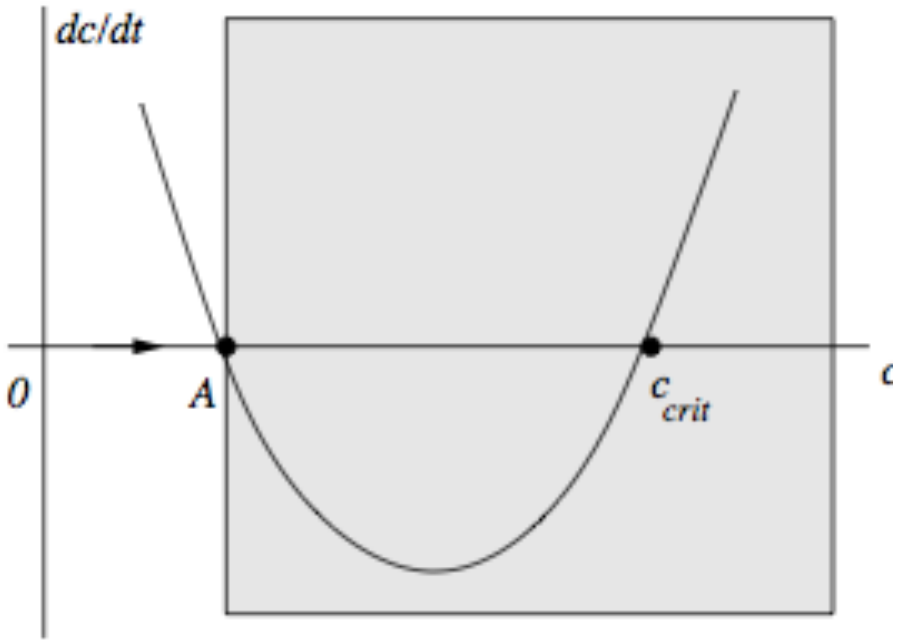
$$\frac{dc}{dt} = k_f (A - c)(c_{crit} - c).$$

$$c_{crit} = \delta / k_f$$



(a)

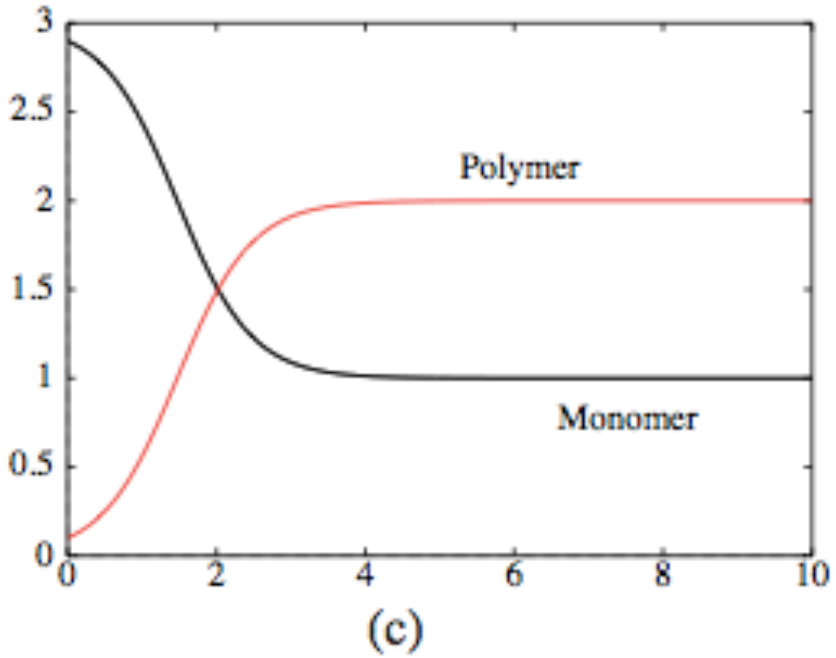
$A > c_{crit}$



(b)

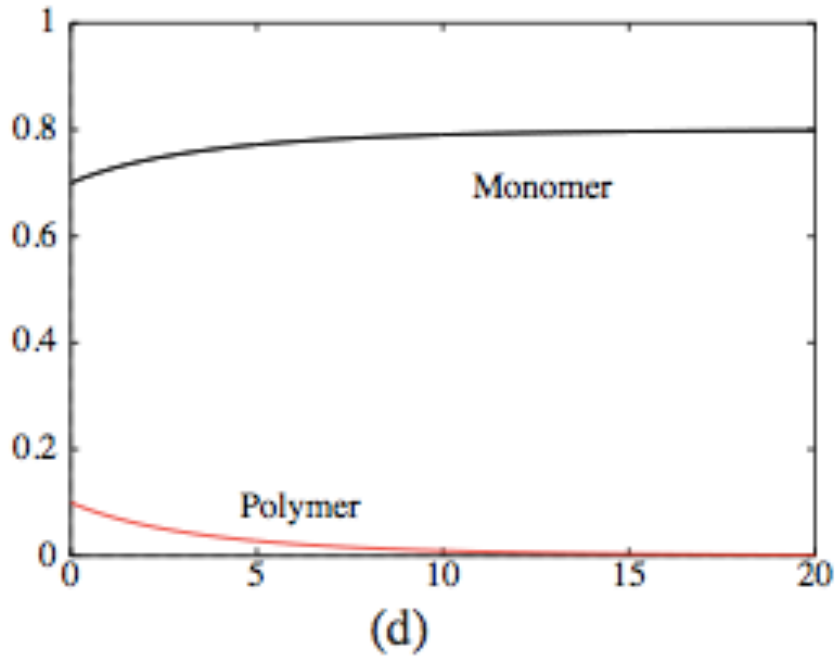
$A < c_{crit}$

Time behaviour



$A > c_{crit}$

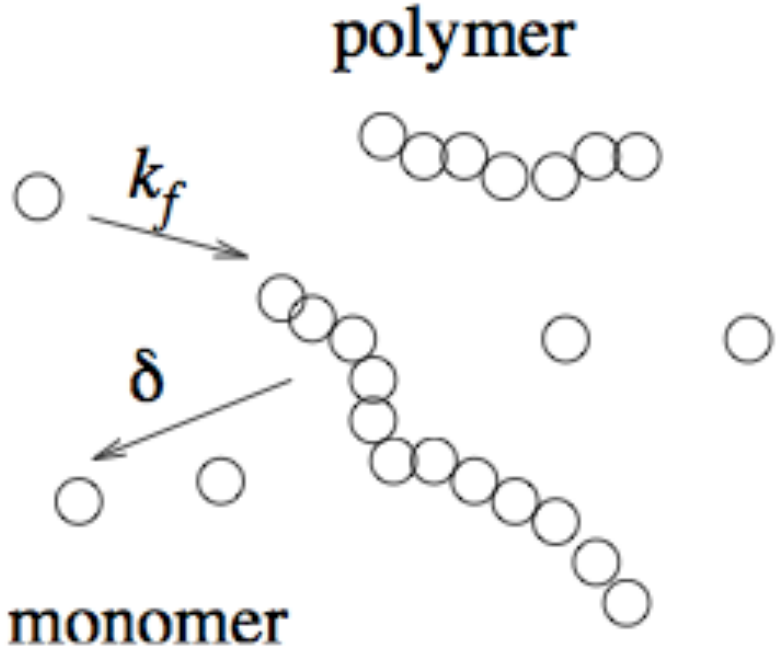
Monomer and polymer equilibrate at constant levels.



$A < c_{crit}$

Only monomer will be left
All polymer disassembles.

(2) Filaments with assembly only at ends and turnover of whole filament



$n =$ Number of filaments (or filament tips)

(assumed constant for now)

Kinetics

$$\frac{dc}{dt} = -k_f cn + \delta F,$$

$$\frac{dF}{dt} = k_f cn - \delta F.$$

Filament disassembles entirely at rate delta

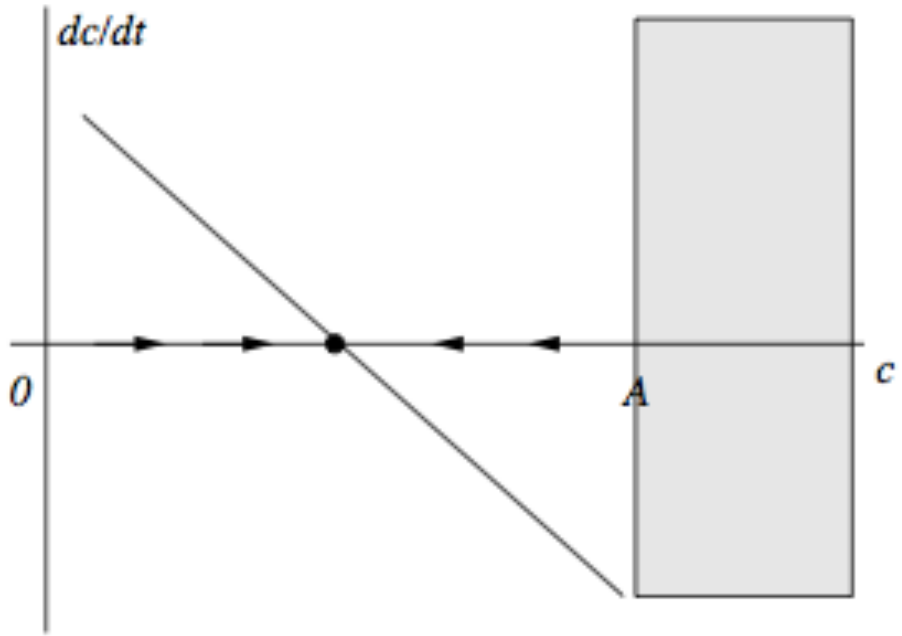
Total $A = c + F$ = constant, eliminate F

$$\frac{dc}{dt} = -k_f cn + \delta(A - c) = \delta A - c(k_f n + \delta).$$

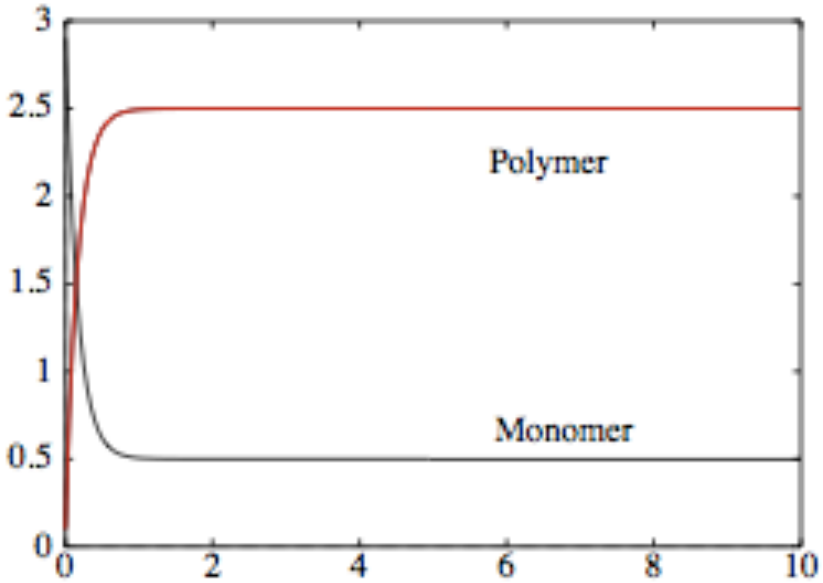
Simulations

```
dc/dt=-kf*c*n +kr*F
dF/dt=kf*c*n -kr*F
param kf=1, kr=1, n=5
init c=2.9, F=0.1
done
```

Predicted behaviour



(a)

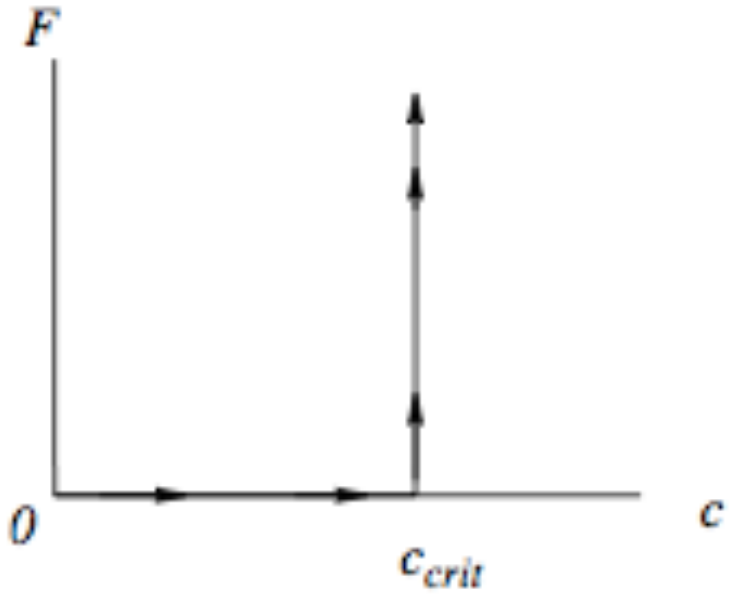


(b)

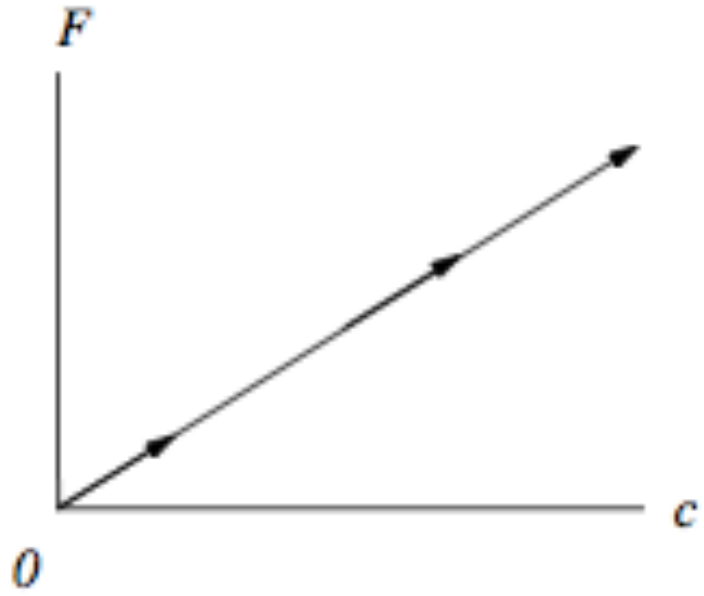
There is always a nontrivial equilibrium level of monomer and polymer

Adding monomers to the mixture

Compare the two cases when the total amount is gradually increased



Type (1)



Type (2)

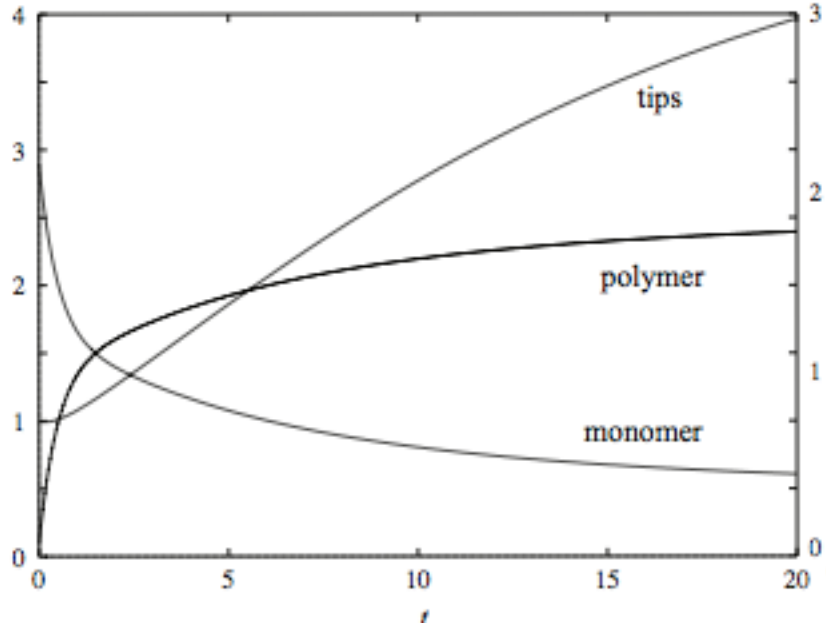
Tips created and capped

$$\frac{dn}{dt} = \phi F - \kappa n,$$

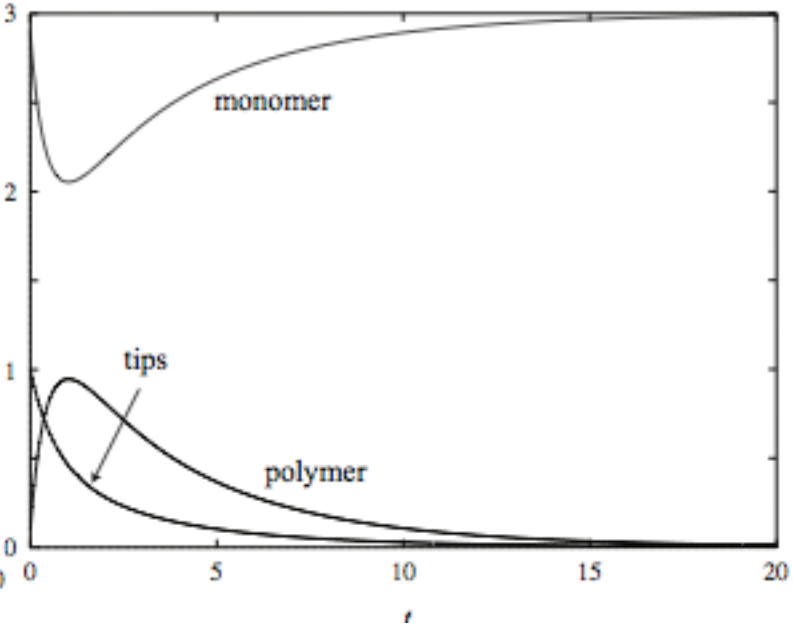
$$\frac{dc}{dt} = -k_f c n + \delta F.$$

Branching and capping

Low capping rate



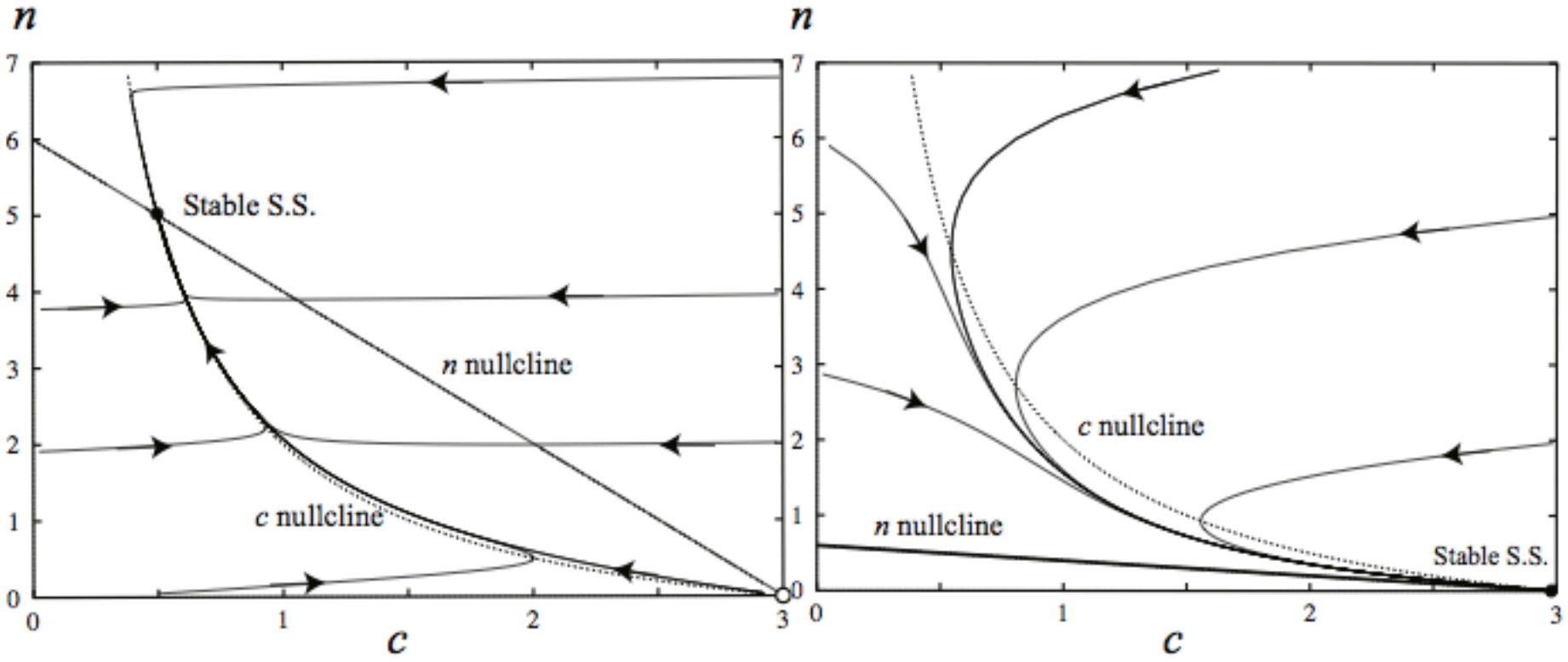
High capping rate



Simulations

```
dc/dt=-kf*c*n +delta*(A-c)
dn/dt=phi*(A-c)-kappa*n
#
aux F=A-c
#dF/dt=kf*c*n -kr*(A-c)
param kf=1, delta=1, kappa=0.1, phi=0.2, A=3
init c=2.9, n=1
@ total=20,xp=c,yp=n,xlo=0,xhi=3,ylo=0,yhi=7
done
```

Phase-plane Behaviour



Low capping rate

High capping rate