Reconfiguration of Production in CSTR Networks: Flexibility of Heterogeneous Setups

Sukanya Balasubramanian, Eric Tatara,
İnanç Birol, Fouad Teymour, and Ali Çinar

Center for Complex Systems and Dynamics
Department of Chemical and Environmental Engineering
Illinois Institute of Technology

AIChE Annual Meeting, Austin, TX, November 7-12, 2004

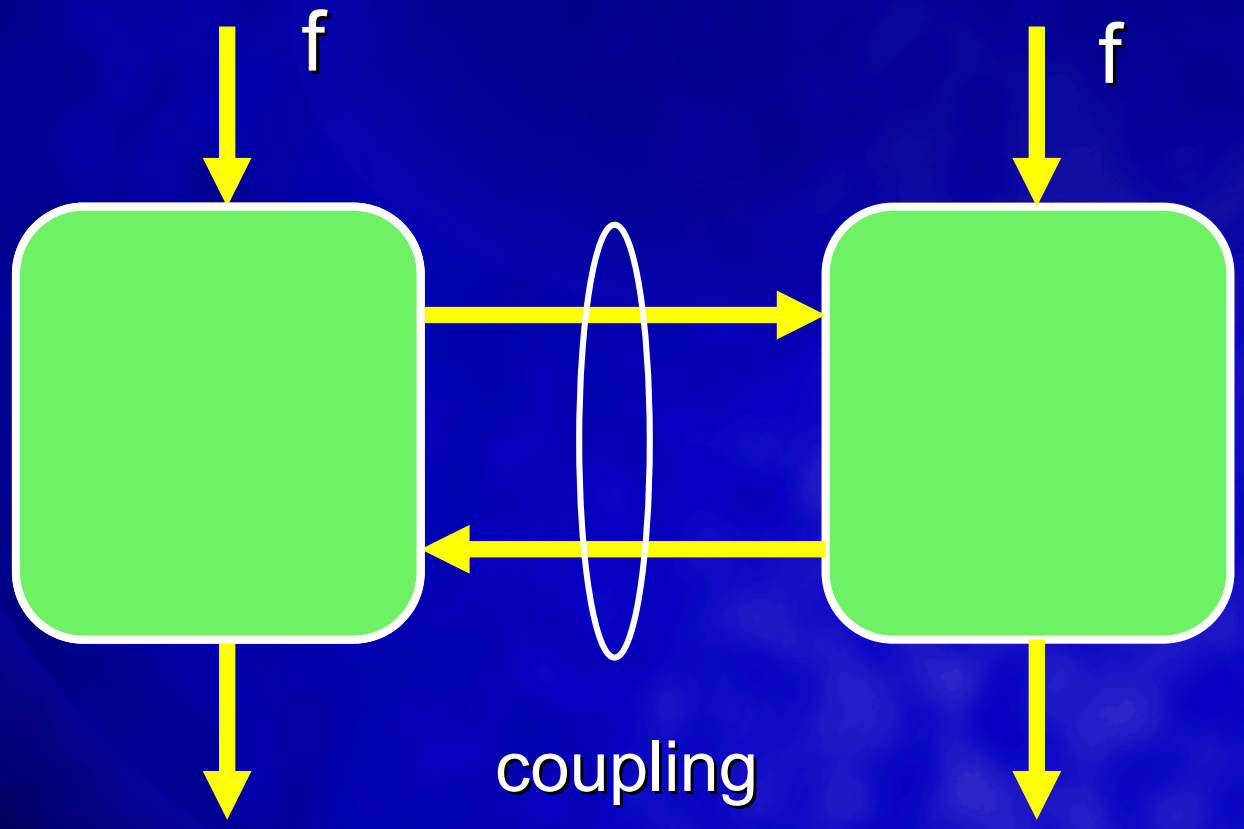
Outline

- Introduction
- Symmetric network feed distribution
- Asymmetric network feed distribution
- Effects of degree of asymmetry
- Analysis of stable regions
- Conclusions

Introduction

- Coupled CSTRs

Locked mode operation

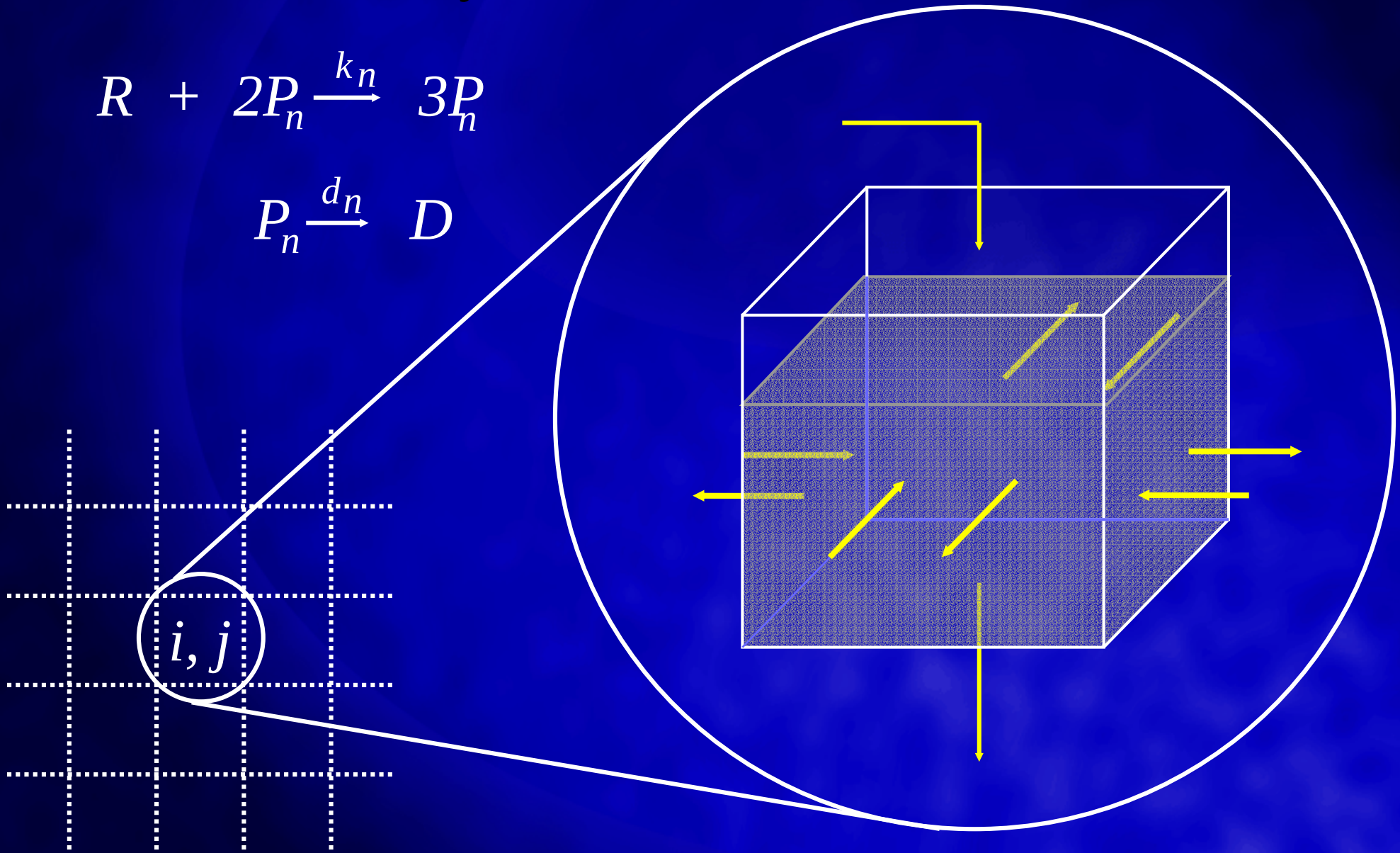


2D Reactor Network

Cubic autocatalysis

$$R + 2P_n \xrightarrow{k_n} 3P_n$$

$$P_n \xrightarrow{d_n} D$$



2D Reactor Network

Cubic autocatalysis

$$R + 2P_n \xrightarrow{k_n} 3P_n$$

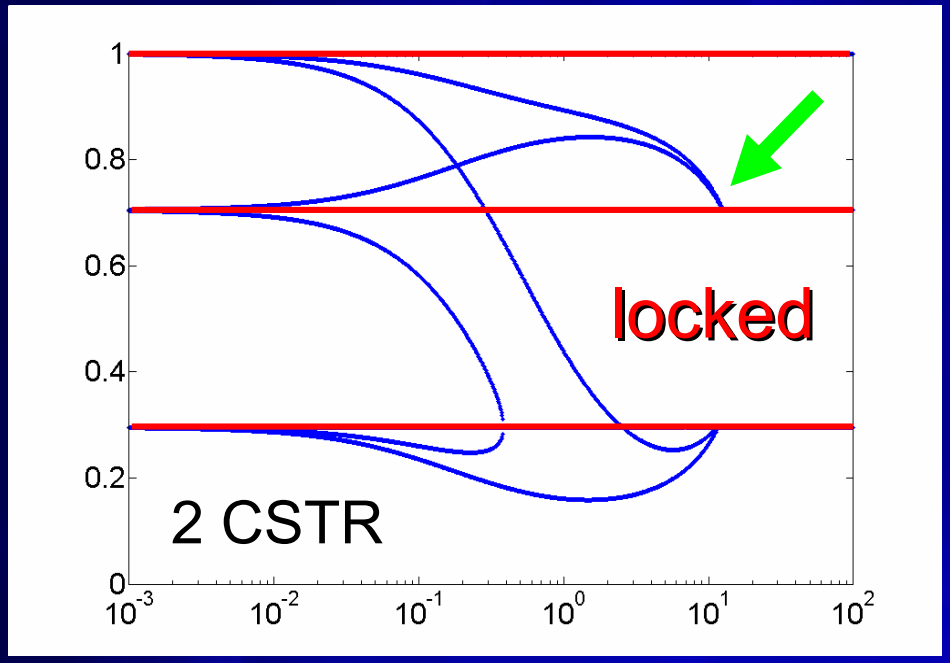
$$P_n \xrightarrow{d_n} D$$

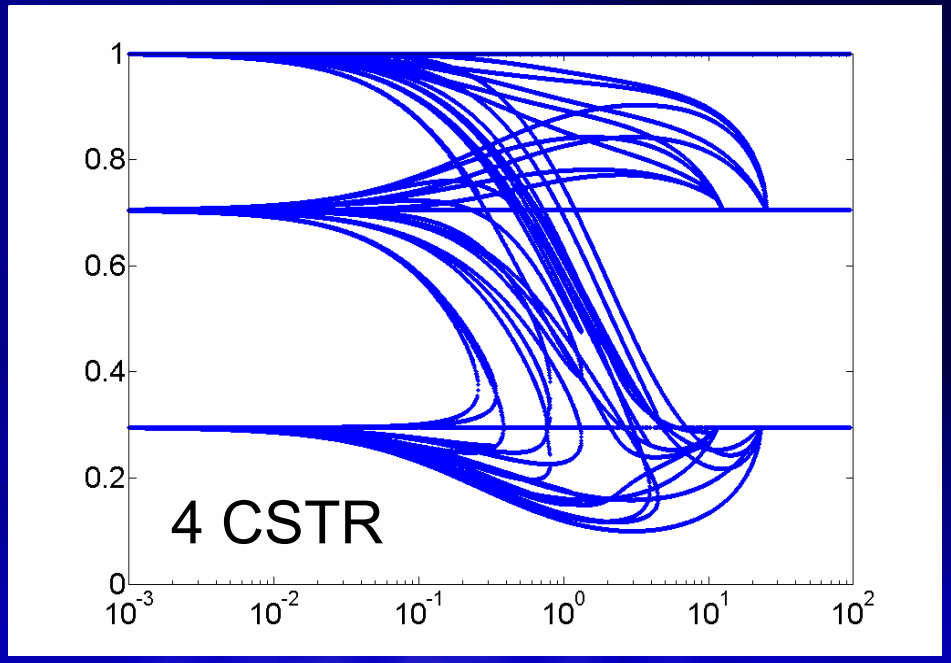
R	resource concentration
R_0	resource concentration in feed
P_n	species n concentration
D	dead species
r_{ij}	R/R_0 in reactor i,j
p_{ijn}	P/R_0 in reactor i,j
k_n	growth rate of species n
d_n	death rate of species n
f	feed flow rate
g	interaction flow rate
t	time

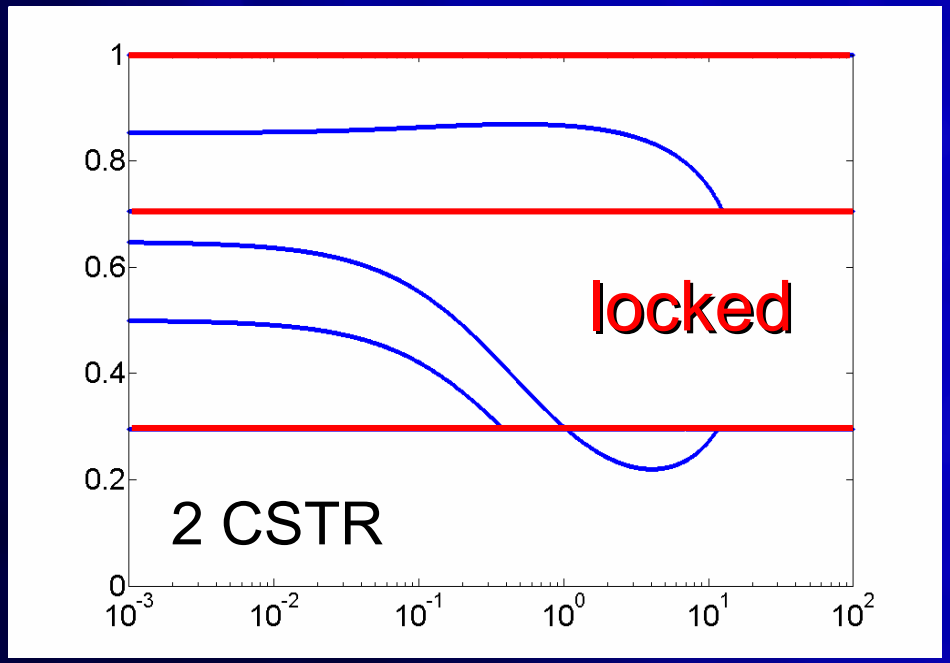
$$\frac{dr_{ij}}{dt} = -\sum_{n=1}^{N} k_n r_{ij} p_{ijn}^2 + f\left(1 - r_{ij}\right) + g\left(r_{i-1,j} + r_{i+1,j} + r_{i,j-1} + r_{i,j+1} - 4r_{ij}\right)$$

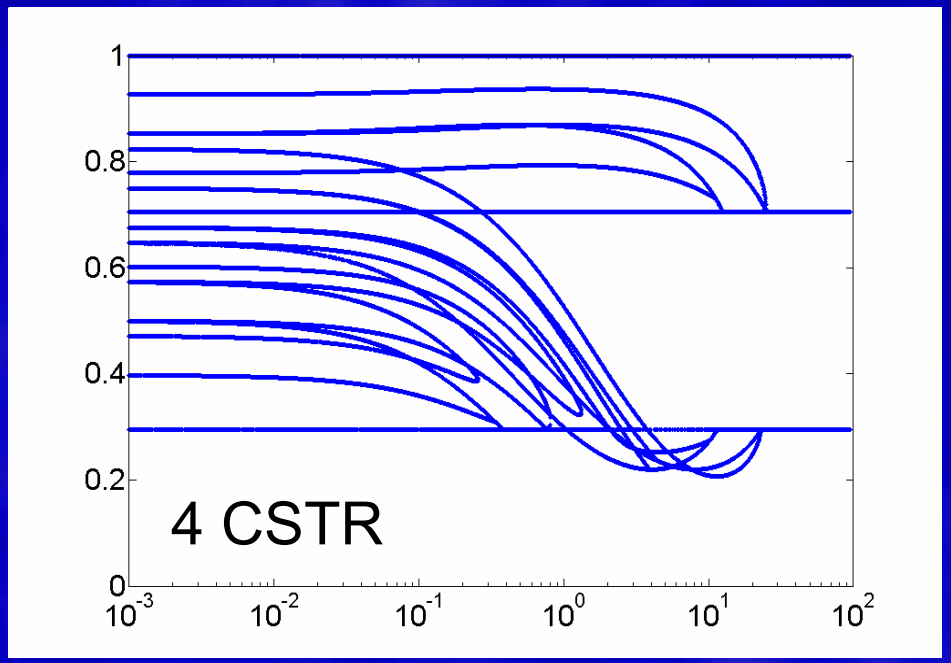
$$\frac{dp_{ijn}}{dt} = k_n r_{ij} p_{ijn}^2 - p_{ijn}\left(f + d_n\right) + g\left(p_{i-1,j,n} + p_{i+1,j,n} + p_{i,j-1,n} + p_{i,j+1,n} - 4p_{ijn}\right)$$

Bifurcation Studies: Uniform feed dist*





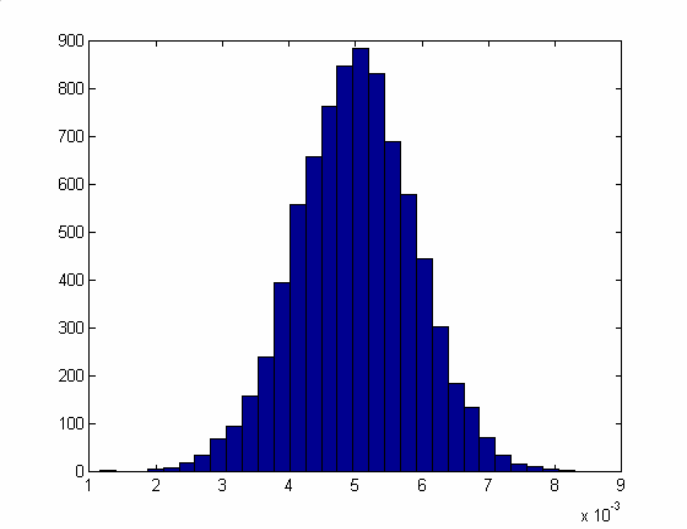




g / f

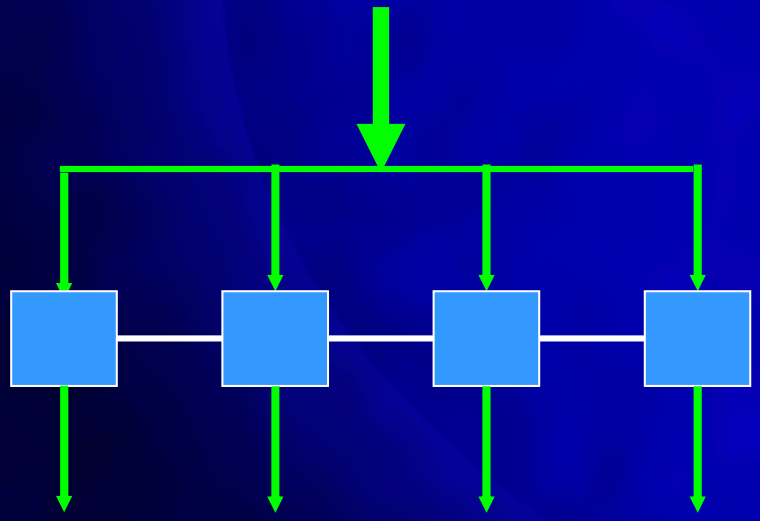
*Tatara, et al 2002,2004

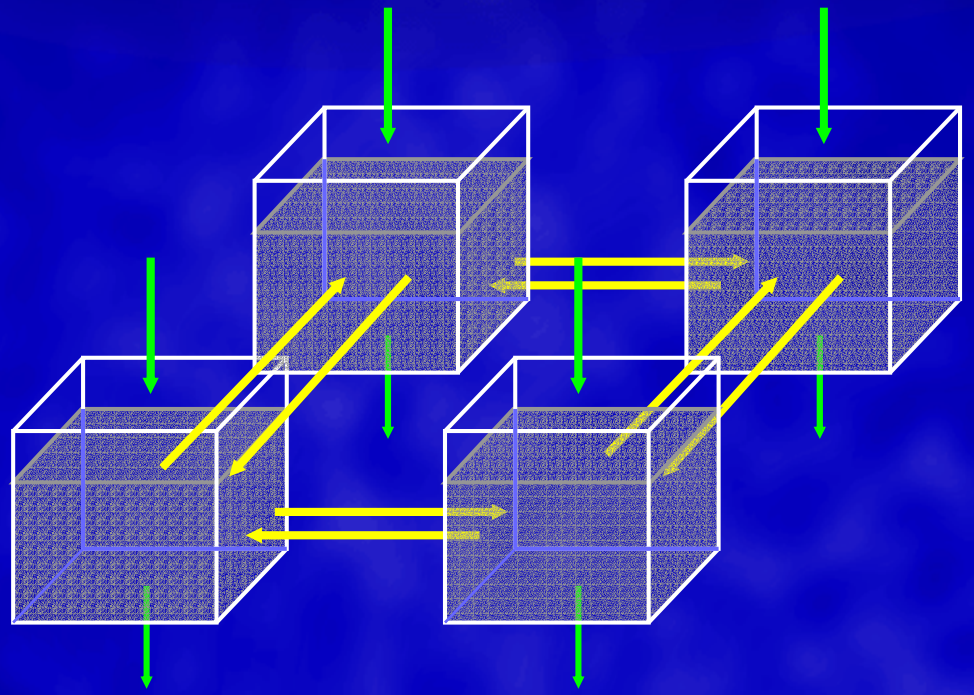
Distribution of Feed Flow Rates



- Flow rates sampled from $N(f,\sigma)$
- Observe effect of σ

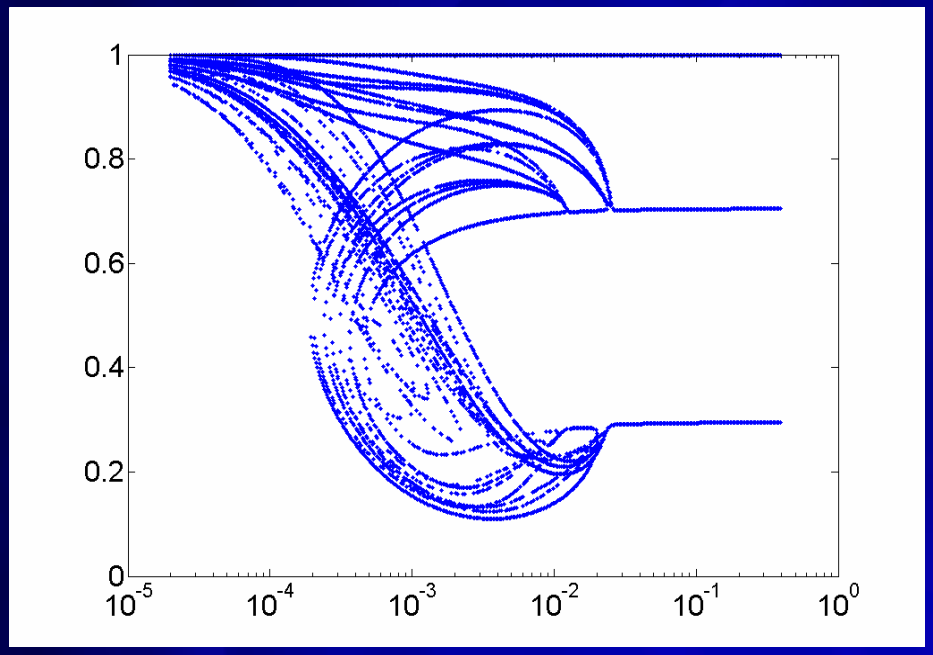
⟹ Degree of heterogeneity

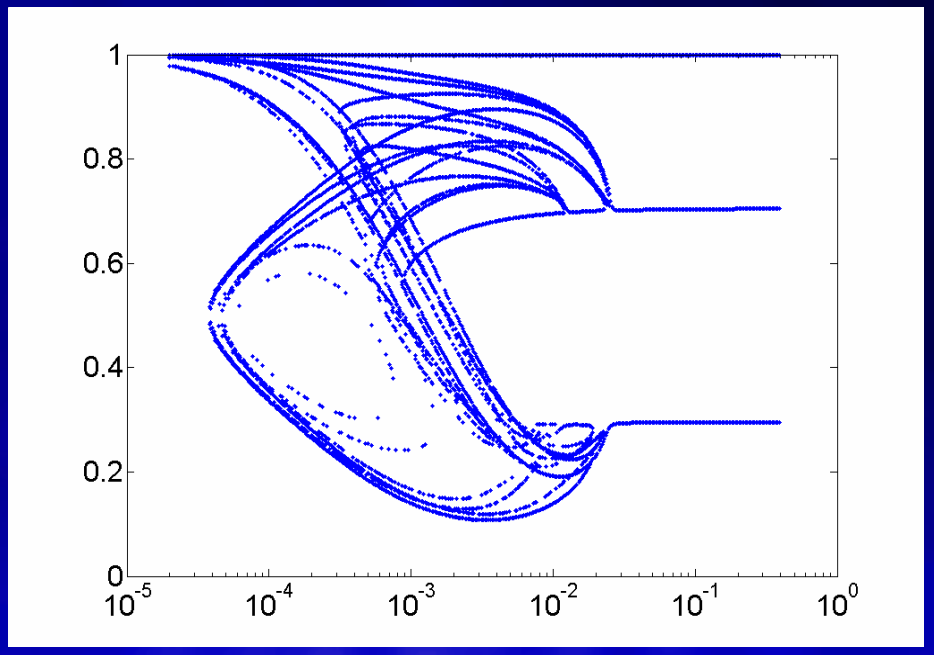


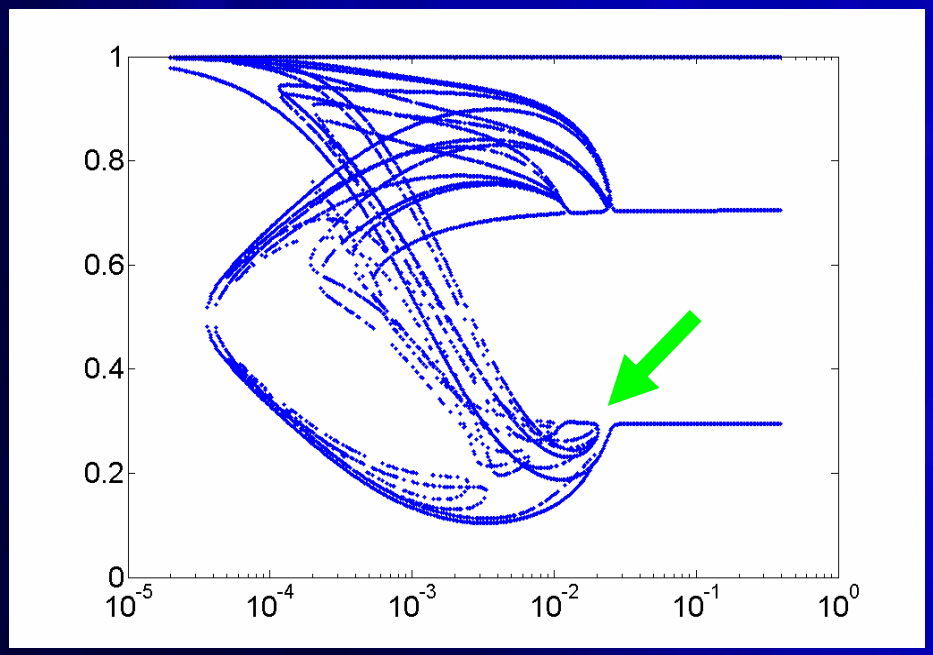


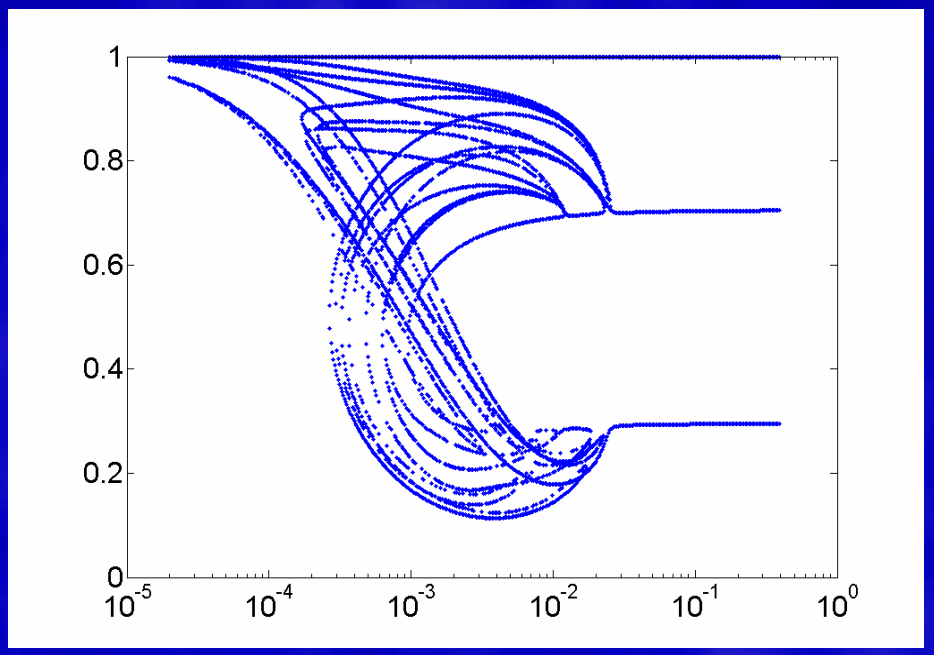
Resource

$f = 0.002,\ \sigma = 0.001$

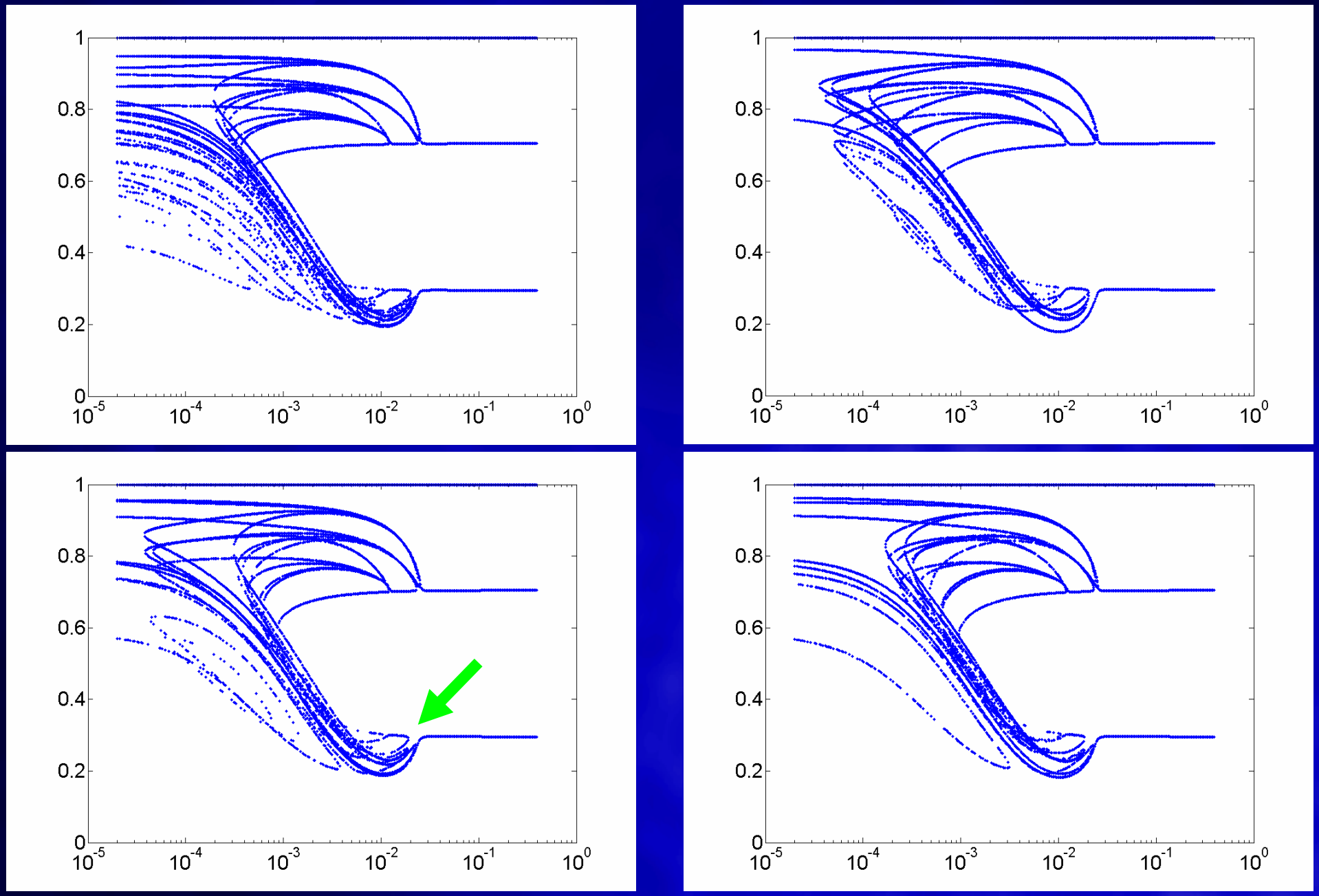






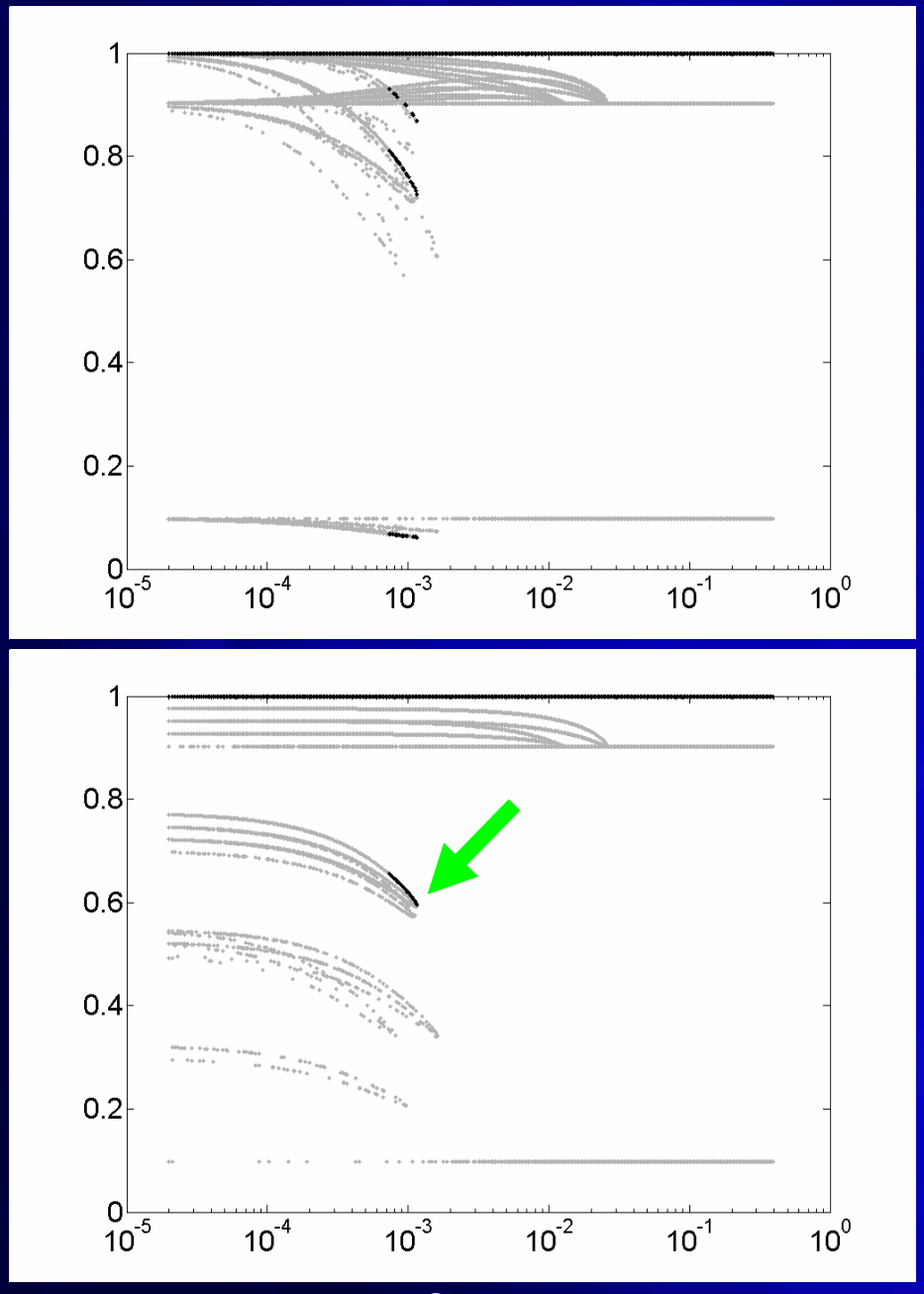


Net Avg Resource $f = 0.002, \sigma = 0.001$



Stable Regions

$f = 0.005$, $\sigma = 0$

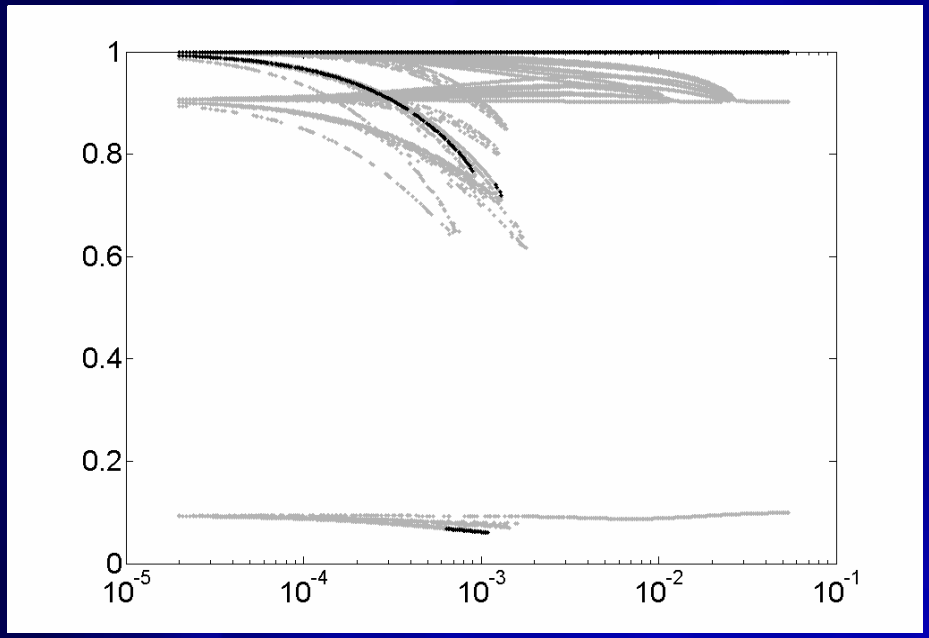


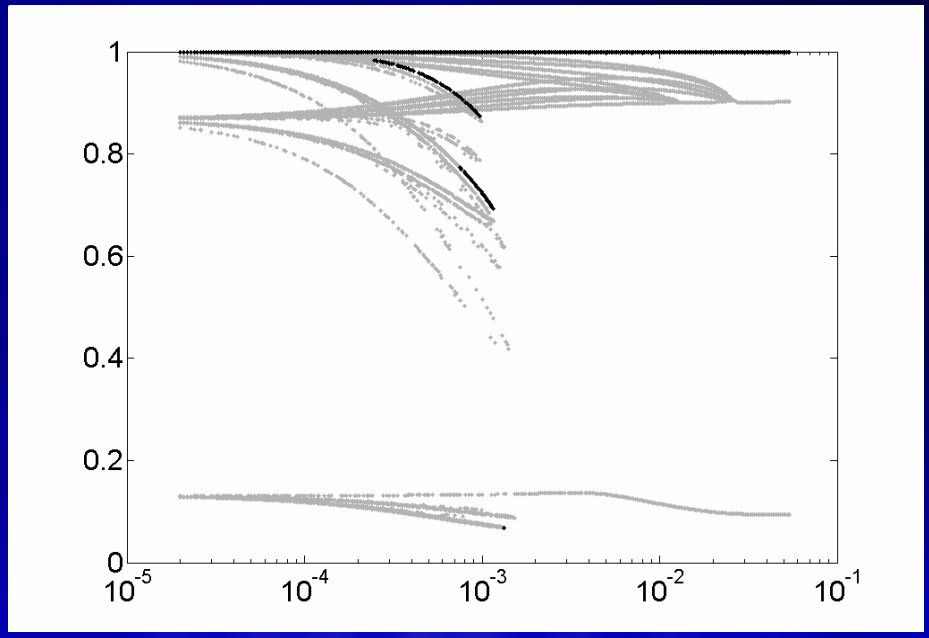
Emergence of stability

Resource 0.001

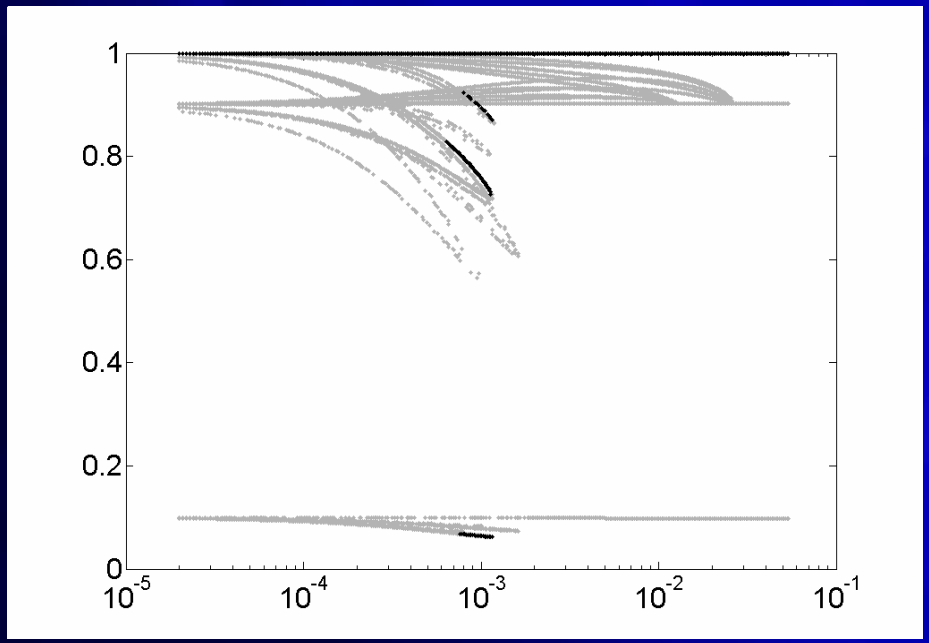
$f = 0.005, \sigma =$

r



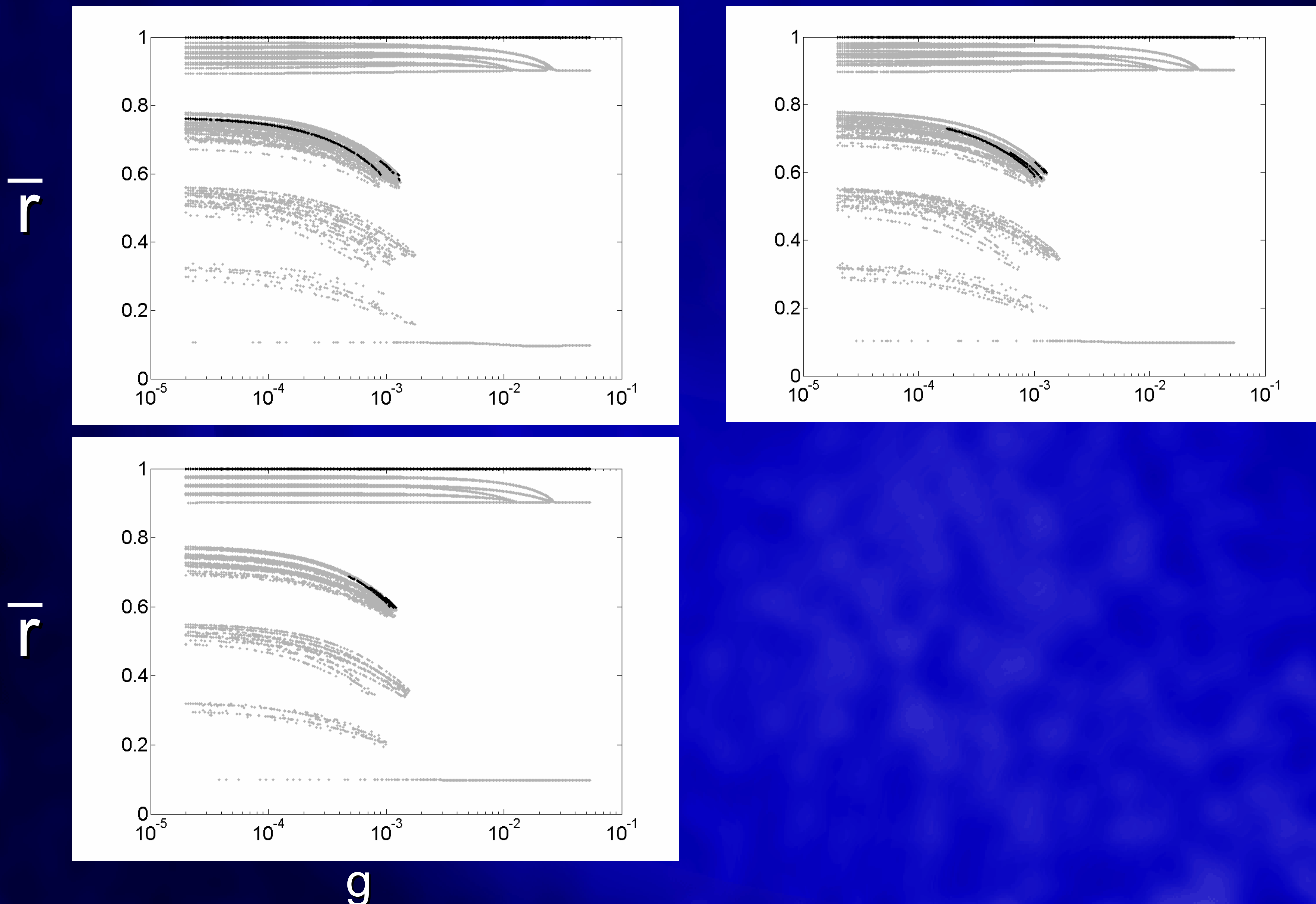


r

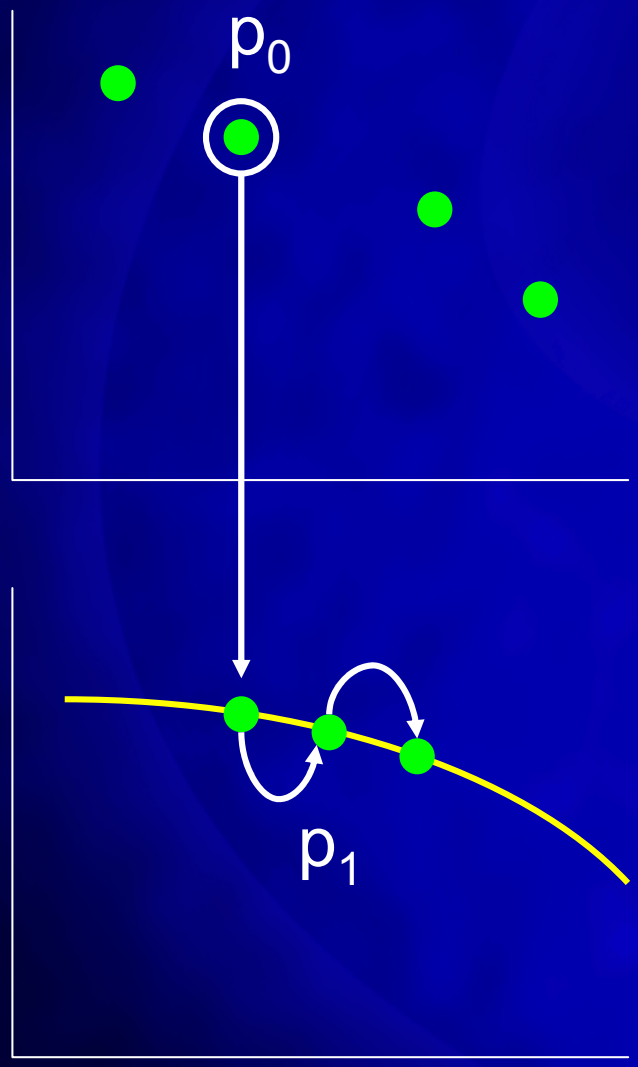


g

Net Avg Resource $f = 0.005, \sigma = 0.001$

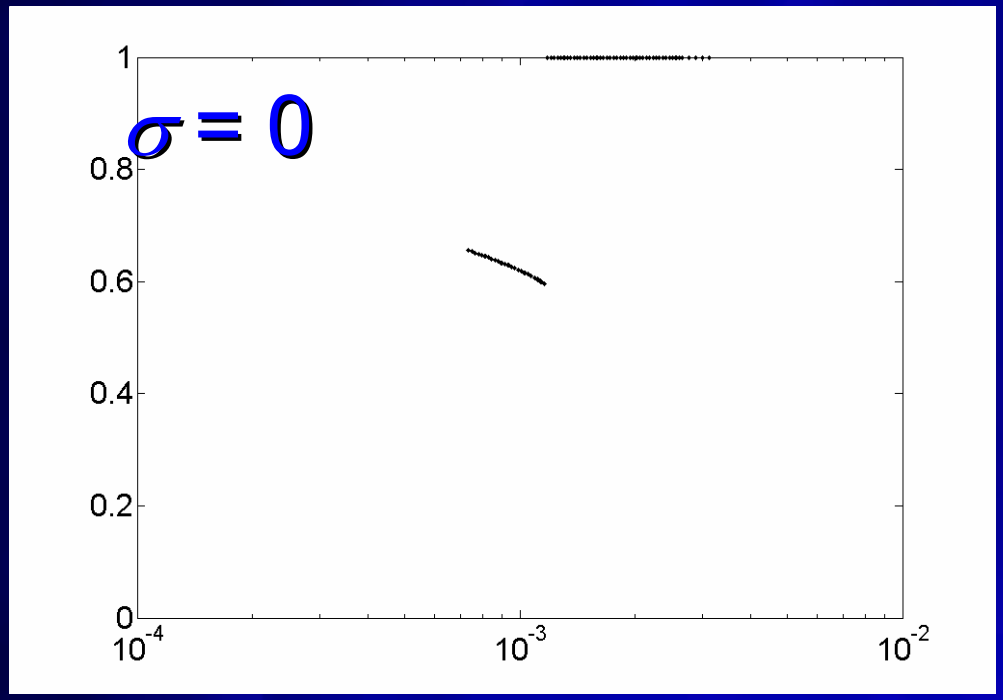


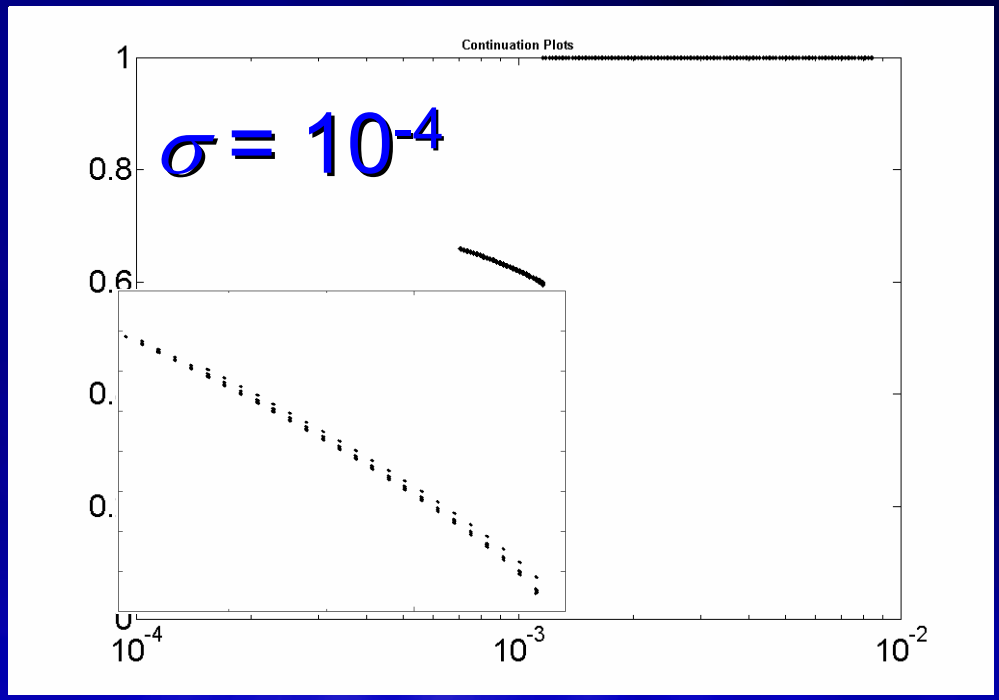
Automated Continuation

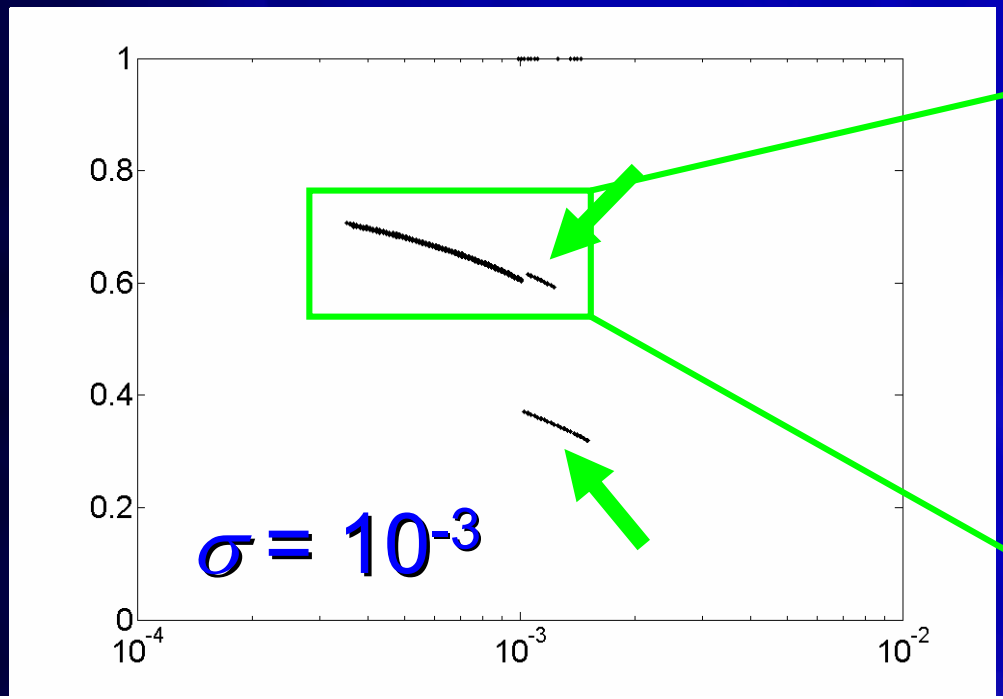


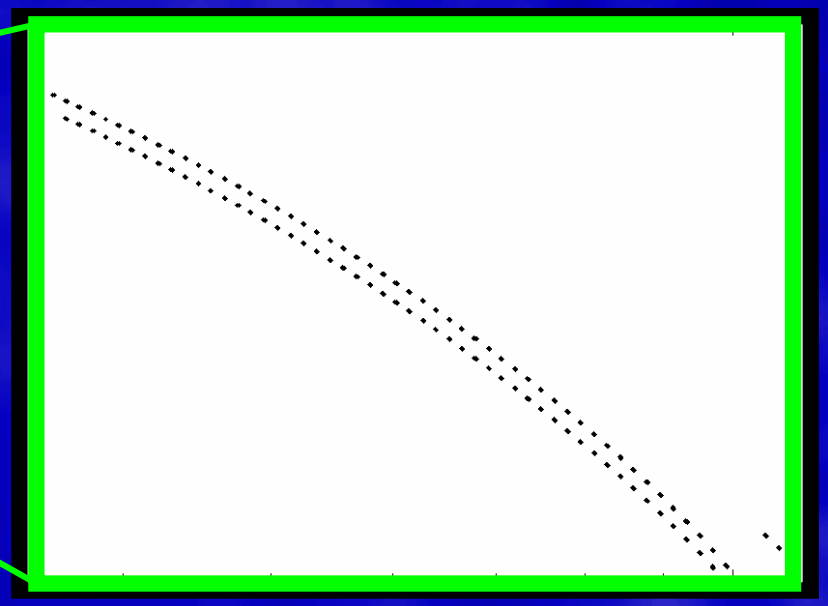
1. Identify stable point p_0
2. Increment bifurcation parameter
3. Use p_0 as initial guess for p_1
4. Solve for p1 (LLNL KINSOL)
5. Test stability of p_1
6. Repeat 1-5 until unstable
7. Reverse direction

Analysis of Stable Regions

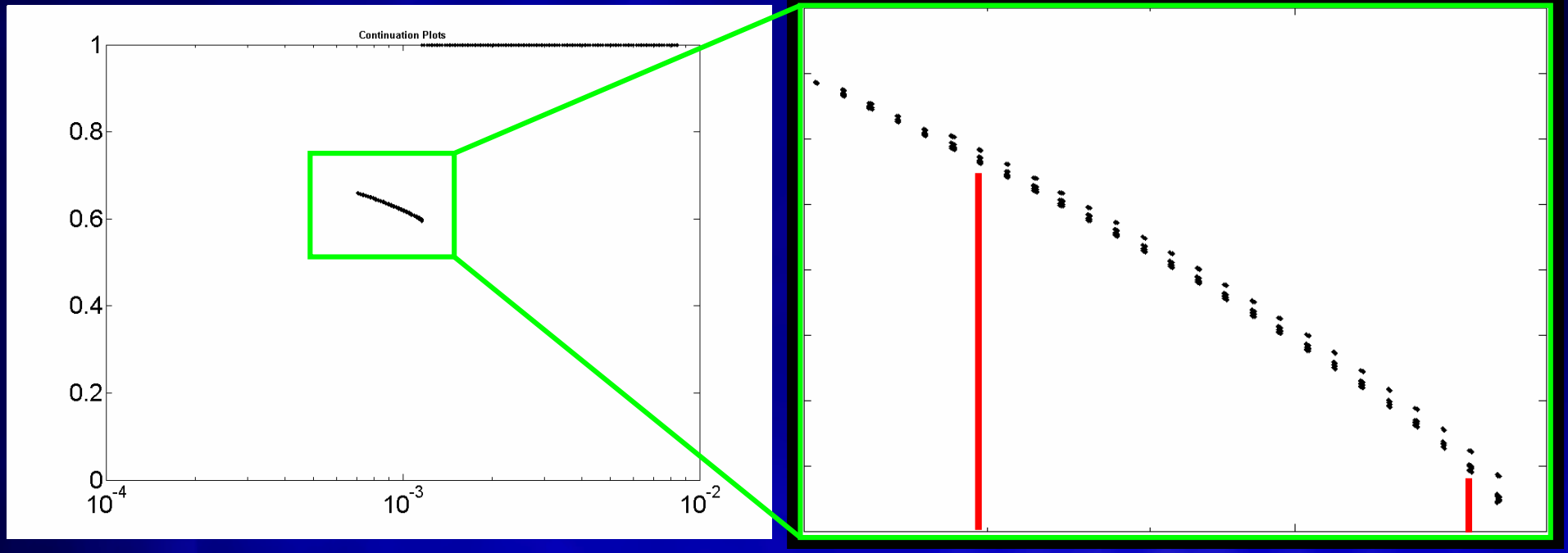




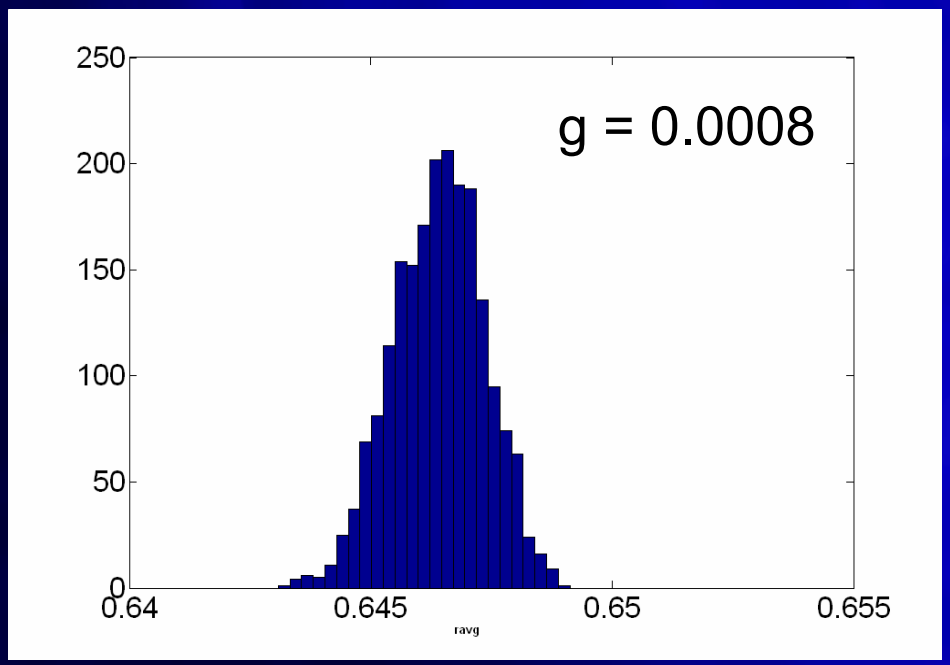


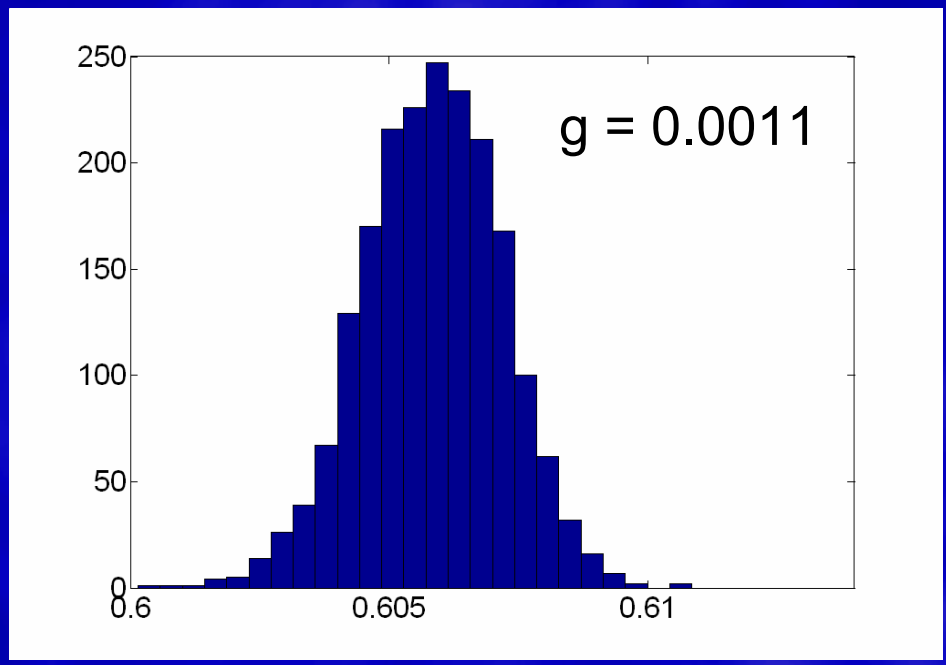


Analysis of Stable Regions, $\sigma = 10^{-4}$



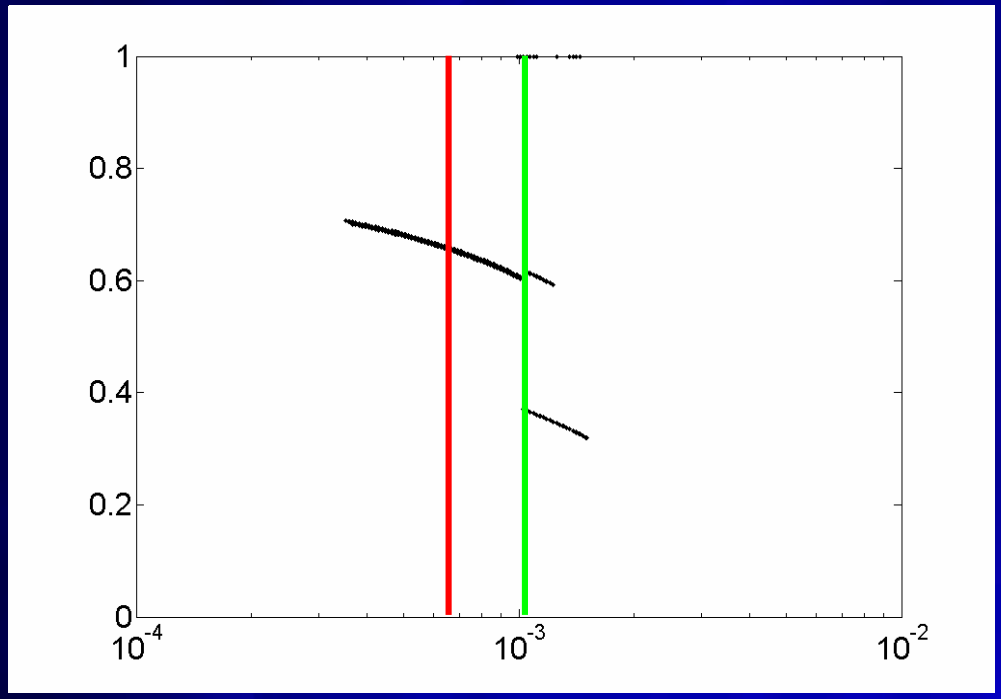
$\bar{r}$

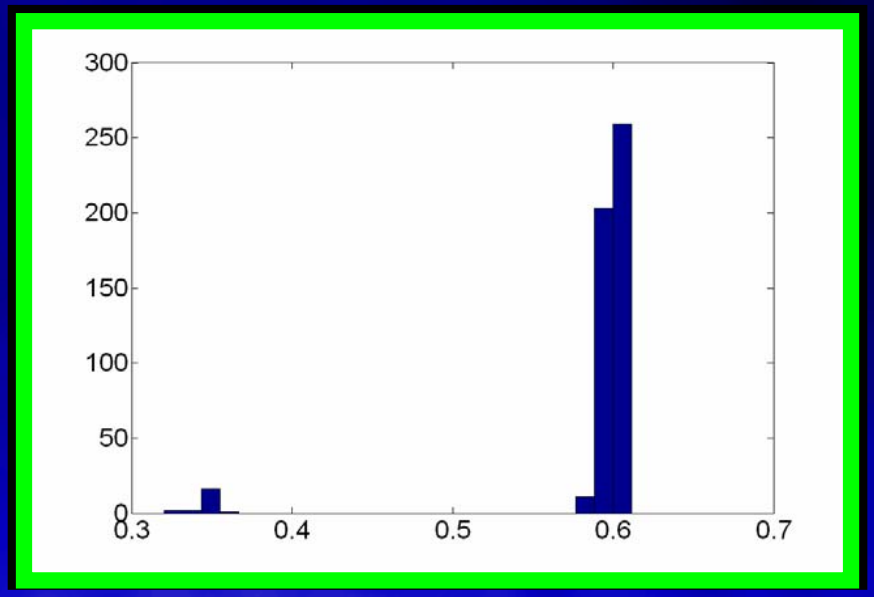


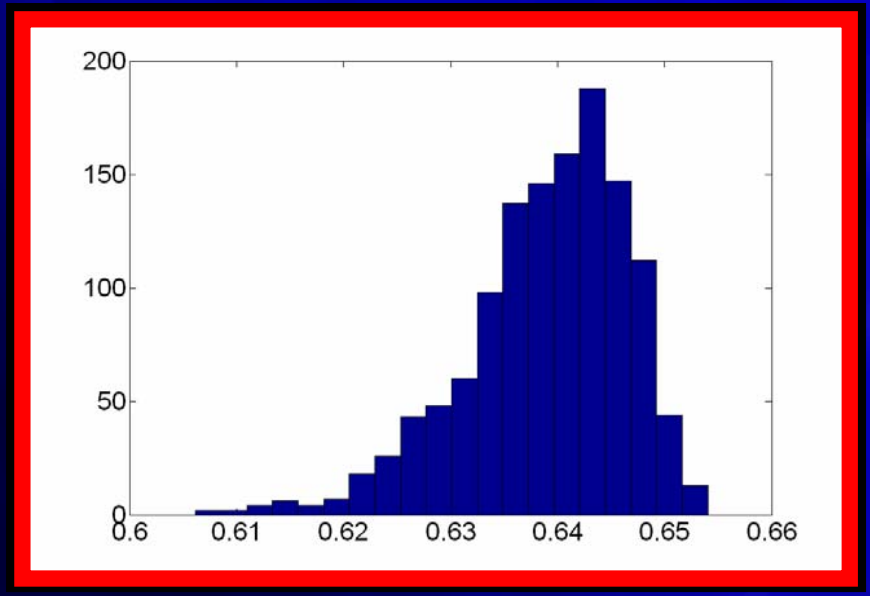


Analysis of Stable Regions, $\sigma = 10^{-3}$

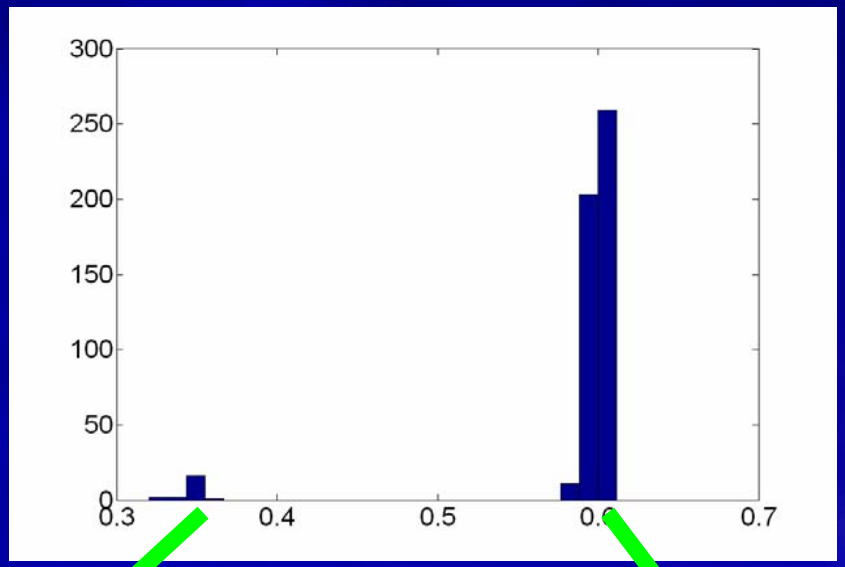
$\bar{r}$

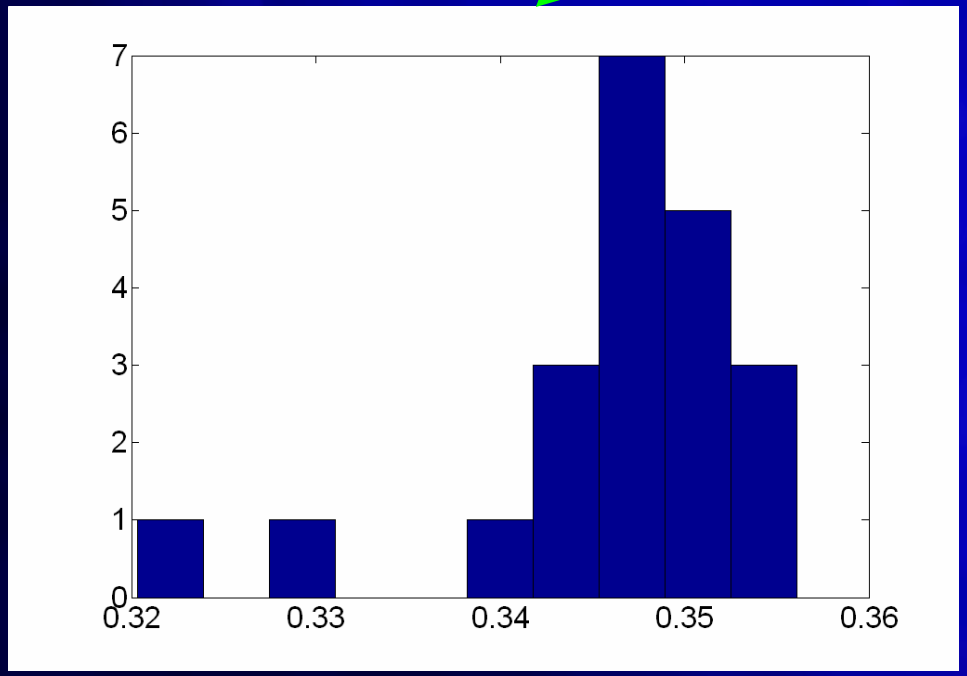


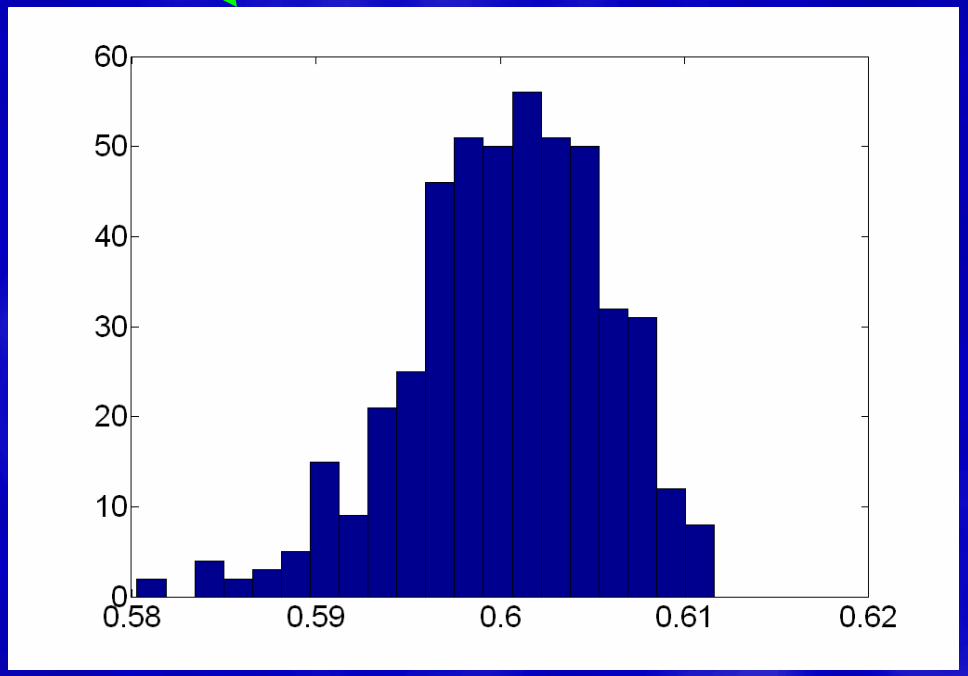




Analysis of Stable Regions, $\sigma = 10^{-3}$







Conclusions

Heterogeneous network configuration

- Suppression of locked mode
- Emergence of new stable points
  - Increased number of states
  - Increased range of stability wrt bifurcation parm

Network operability and flexibility

- Close proximity of states

Natural systems and evolutionary diversity

Contact

Prof. Ali Cınar	cinar@iit.edu
Prof. Fouad Teymour	teymour@iit.edu
Prof. Inanc Birol	birol@iit.edu
Eric Tatara	tataeri@iit.edu
Sukanya Balasubramanian	balasuk@iit.edu

Center for Complex Systems and Dynamics
Department of Chemical & Environmental Engineering
Illinois Institute of Technology
10 W 33rd Street
Chicago, IL 60616
tel : (312) 567 3040
fax : (312) 567 8874

www.chee.iit.edu