Autocatalytic species competition in a heterogeneous environment

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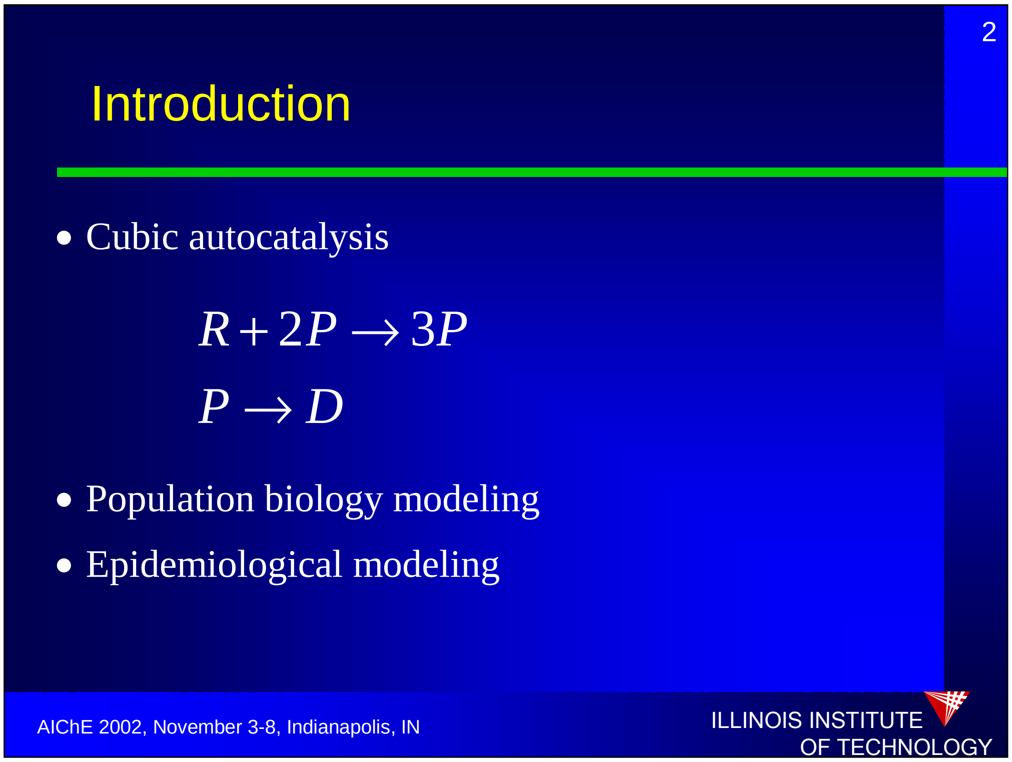


The system of study is the cubic autocatalytic reaction

Cubic autocatalysis can be used to model biological systems in which species reproduce sexually.

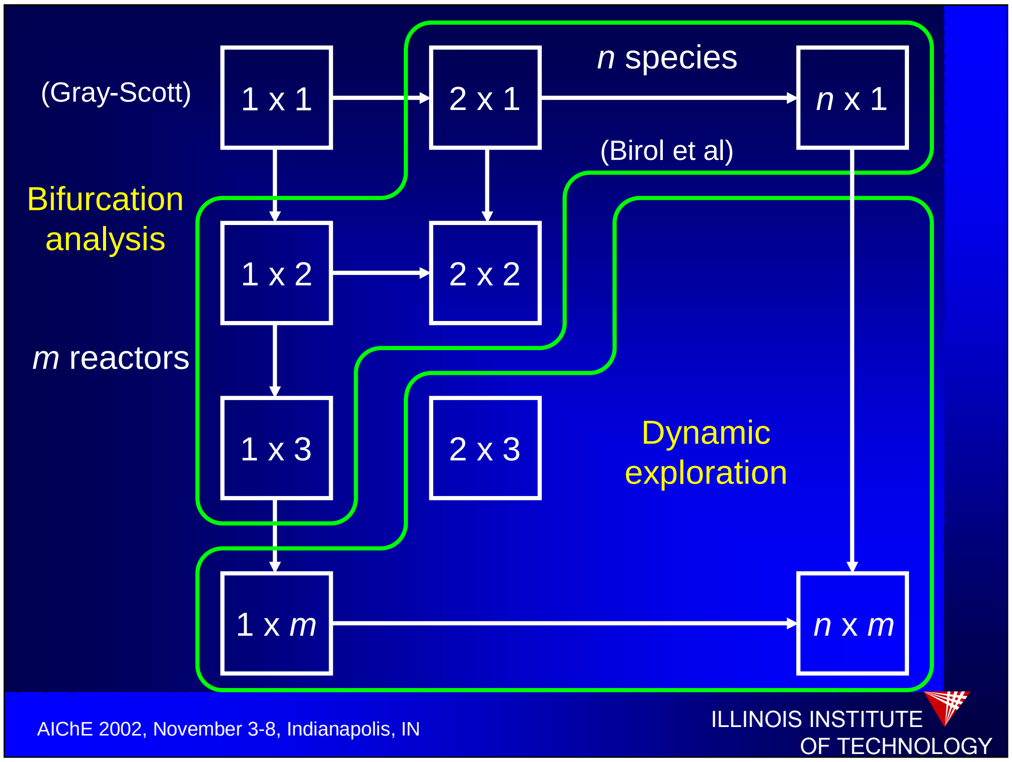


Diagram of possible reactor network configurations

The initial work by Gray and Scott (1983,1984) focused on:

- single CSTR
- single autocatalytic specie
- multiplicity in the form of isolas and mushrooms

In a series of papers, Birol et al (2000,2002) have examined:

- n species in a single CSTR
  - Unstable interaction isola
  - coexistence is not possible
  - limit cycles
- two species in 2 and 3 CSTRs
  - introduction of heterogeneity
  - emergence of new stable steady states
  - number of steady states increase exponentially with problem size
  - strange attractor

Small systems are either analytically tractable, or solved with bifurcation analysis.

The purpose of this work is to investigate intermediate and larger systems via:

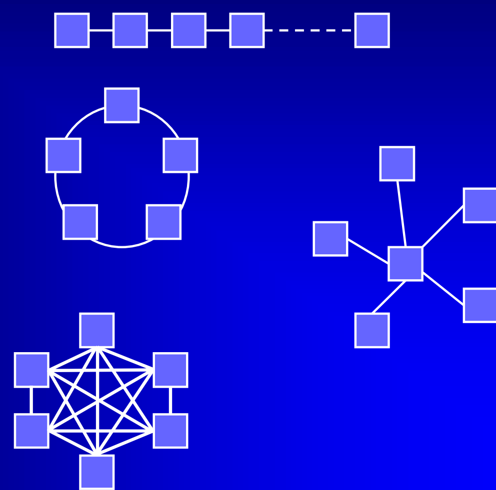
- bifurcation analysis, although analysis of dense bifurcation diagrams is difficult
- dynamic exploration

- establish a relationship between behavior in small and large networks

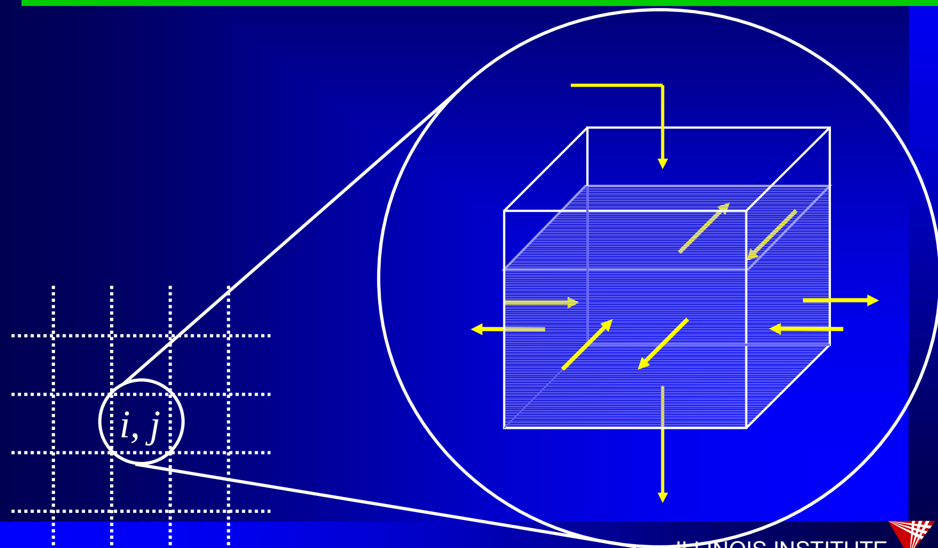
- Phase locking: strong coupling
- Quasi-periodicity: weak coupling
- Traveling waves

Reactor Networks

- Linear
- Ring
- Star
- Hopfield



2D Reactor Network



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2D Reactor Network

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

$$P_n \xrightarrow{d_n} D$$

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

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

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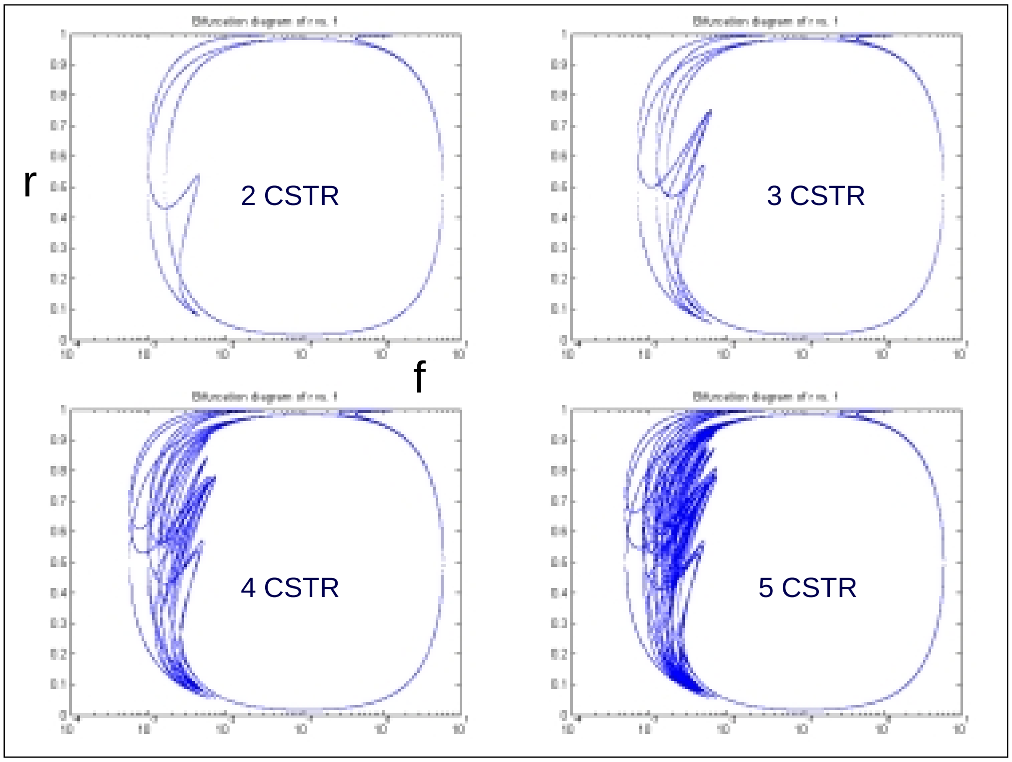
R0: resource concentration in the feed
R: resource concentration r: dimensionless resource = R / R0
P: species n concentration p: dimensionless species = P / R0
D: 'dead' species t: dimensionless time = t'*(R0)^2
V: reactor volume d: dimensionless death rate = d' / (R0^2);
F: feed rate f: dimensionless feed rate = F / (V*R0^2)
G: interconnection flow rate g: dimensionless interconnection flow rate = G / (V*R0^2)

The change in dimensionless resource concentration is determined by

1. The consumption of resource by the n species,
2. The net outflow of resource by the feed flow
3. The net outflow of resource by the interconnection flows

The change in dimensionless species concentration is given by:

1. The production of species
2. The net outflow of species due to feed and death
3. The net outflow of species due to interconnection flows



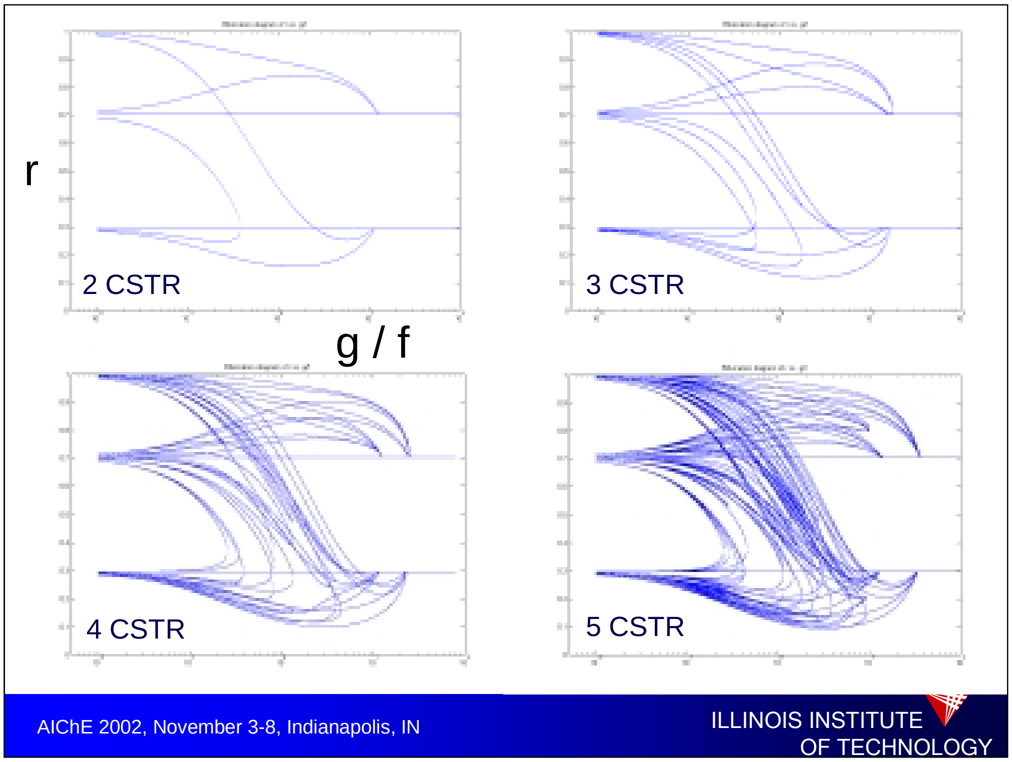
Bifurcation diagrams of resource concentration (in all reactors) vs flow rate, hosting a single species.

Top left: 2 CSTR ring network
Top right: 3 CSTR ring network
Bottom left: 4 CSTR ring network
Bottom right: 5 CSTR ring network

With the increasing size of the network, the number of steady states increases as does the range of interconnection flow rates that allow the species to survive.

The emergent behavior is evident by the fact that the network behavior is is more complex than the sum of the individual units.

k1 = 25, d1 = 0.1, g = 0.002



Bifurcation diagrams of resource concentration (in all reactors) vs g/f hosting a single species.

Top left: 2 CSTR ring network

Top right: 3 CSTR ring network

Bottom left: 4 CSTR ring network

Bottom right: 5 CSTR ring network

With the increasing size of the network:

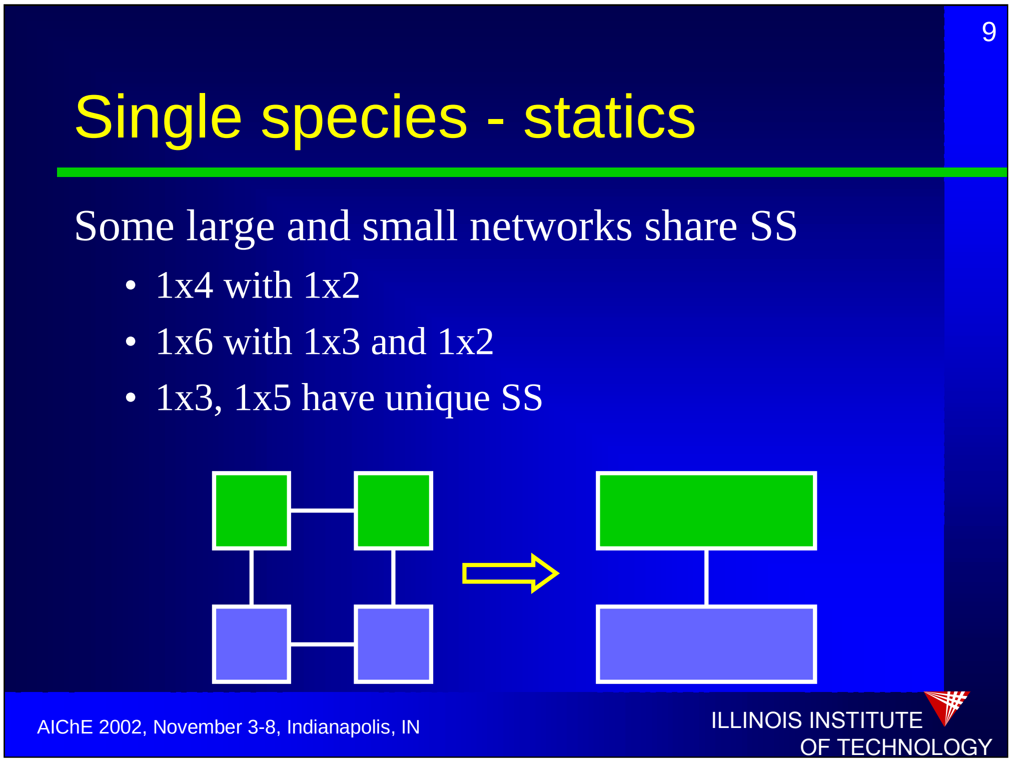
the number of steady states (SS) increase

the range of interconnection flow rates that allow the species to survive increase.

The 4 CSTR network shares SS with the 2 CSTR network

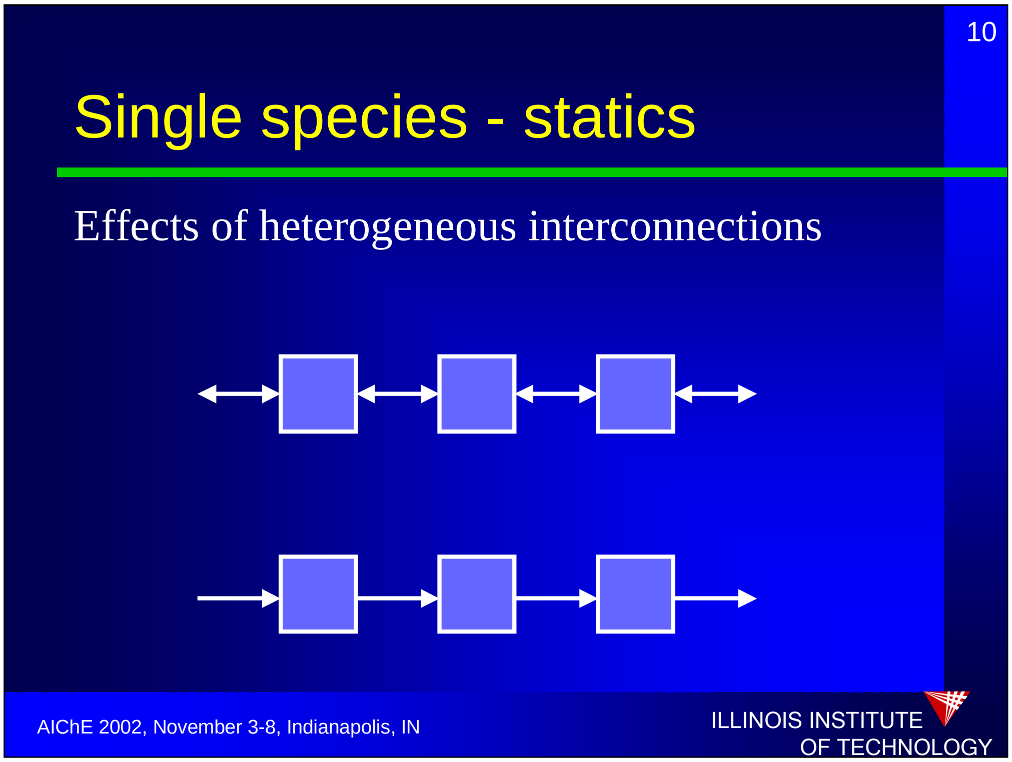
The 6 CSTR network shares SS with the 2 and 3 CSTR networks

k1 = 25, d1 = 0.1, f = 0.002



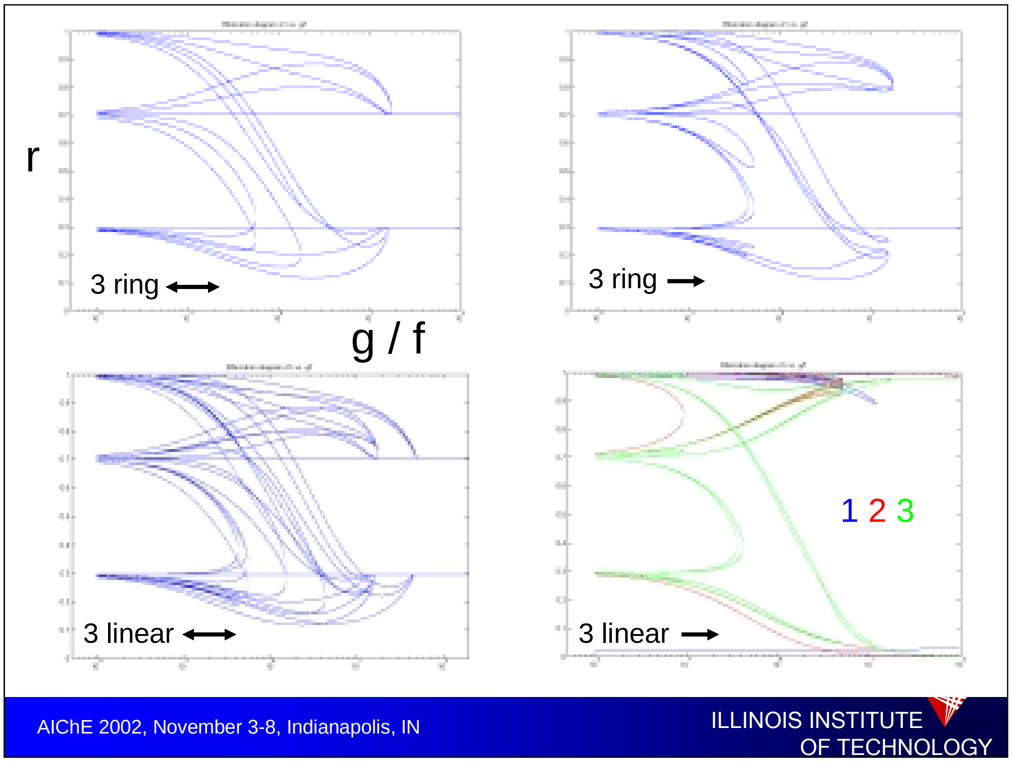
Networks that are multiples of smaller networks share steady states (SS)

For example, a 4 CSTR network can also represent a 2 CSTR network



The previous diagrams represent systems in which the interconnection flow rate are equal for the entire network.

Manipulating the interconnection flow rates is a means to introduce heterogeneity.



Bifurcation diagrams of resource concentration vs g/f hosting a single species.

Top left: 3 CSTR ring network

Top right: 3 CSTR ring network with interconnection flow in one direction only

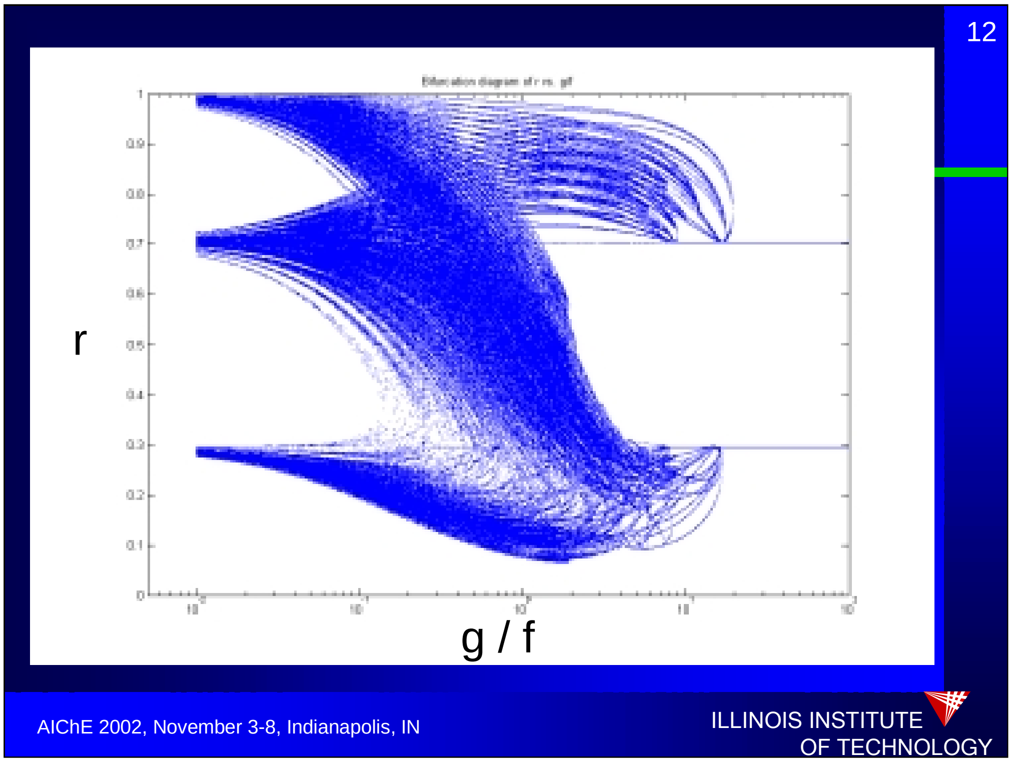
Bottom left: 3 CSTR linear network

Bottom right: 3 CSTR linear network with interconnection flow in one direction only

The horizontal lines are steady states (SS) in the single CSTR system.

With the increasing heterogeneity of the network, the number of SS increase as does the range of interconnection flow rates that allow the species to survive. k1 = 25, d1 = 0.1, g = 0.002

In the last case, the linear network with flow in one direction, the SS do not approach the single CSTR as the interconnection flow rate is increased. Additionally, each CSTR now has unique SS. The feed rate to the first reactor, f1 is different from from the rest of the network to ensure that f1 > g, since the first reactor has only one input via the feed. k1 = 25, d1 = 0.1, f = 0.002, f1 = 0.2.

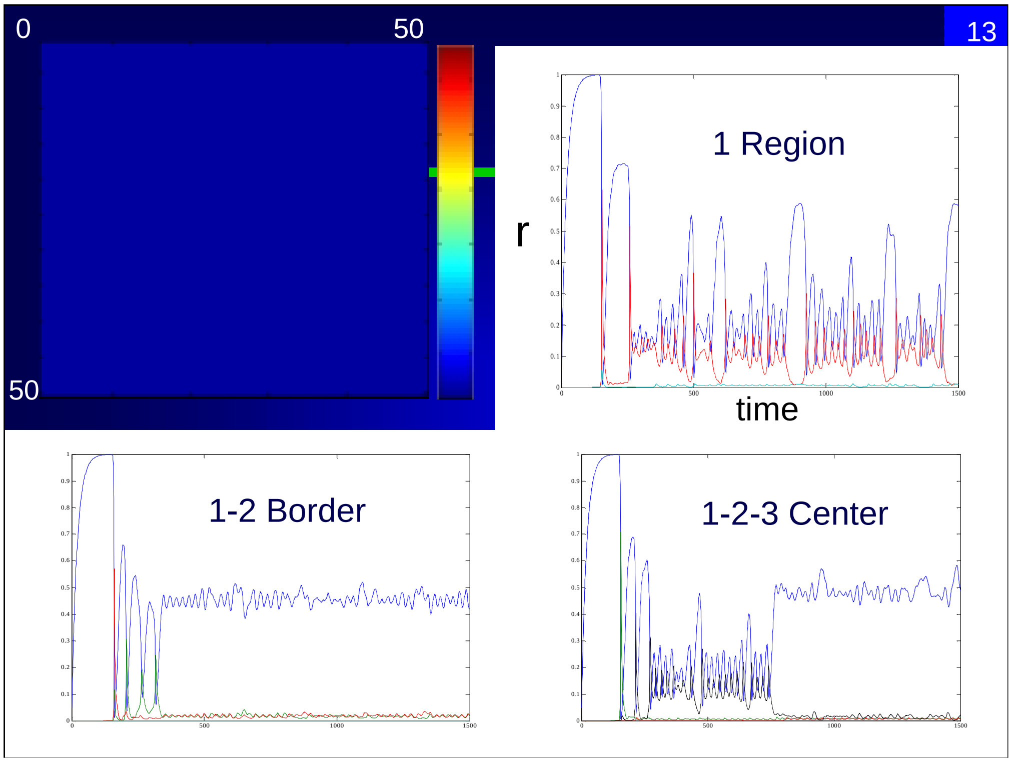


Bifurcation diagrams of resource concentration vs g/f hosting a single species.

3 x 3 2D network with toroidal BCs

In only a relatively small system, it is already evident that the steady states begin to form a continuum between the maximum and minimum concentrations

k1 = 25, d1 = 0.1, f = 0.002



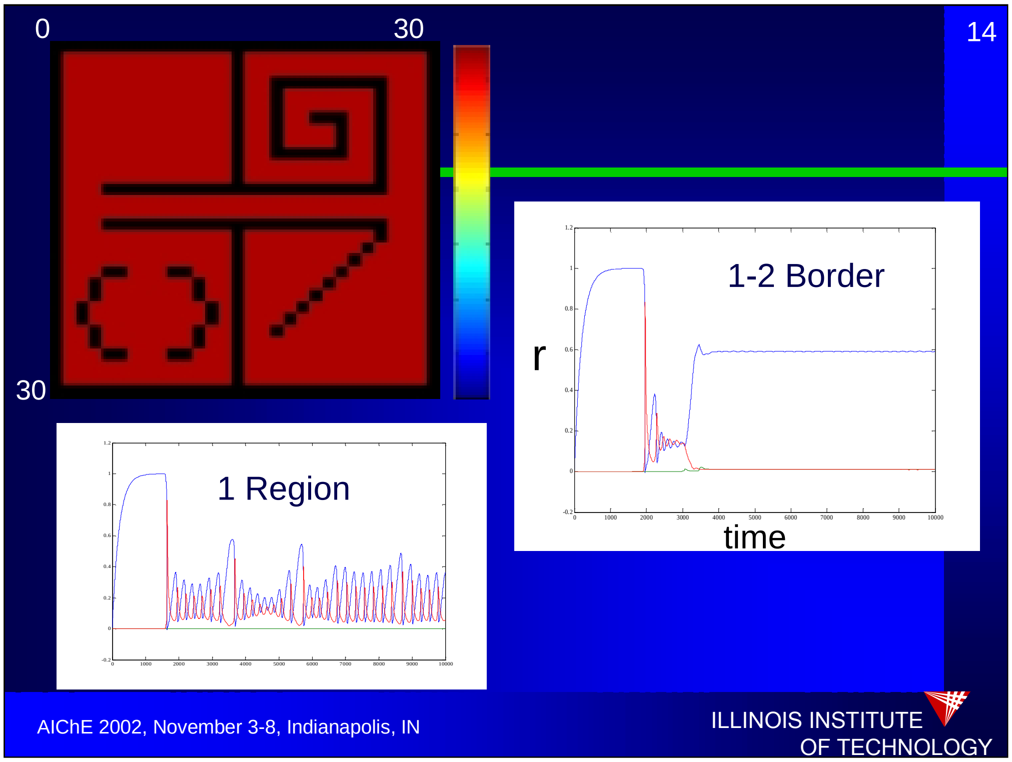
Simulation of 50 x 50 network with 3 species.

The competing species are nearly identical with respect to growth and death rates.

Initially, the species are introduced to the network via a pulse input into a single reactor (for each species).

Each species is sustainable in the region near the pulse input and exhibits behavior that includes steady state, limit cycles, quasi-periodicity, and chaos (top right).

The border between species regions contains reactors in which no species is sustainable.



Simulation of 30 x 30 network with 2 species

The two competing species are nearly identical with respect to growth and death rates.

Barriers are simulated using dead reactors – no volume or flow rates

Initially, the species are introduced to the network via a pulse input into a single reactor (for each species).

Each species is sustainable in the region near the pulse input and exhibits behavior that includes steady state, limit cycles, quasi-periodicity, and chaos (bottom).

The border between species regions contains reactors in which no species is sustainable.

Initially, species 2 spears to settle on a steady state (right).

After species 1 increases slightly, species 2 falls to to a very low state with species 1

Conclusions

- Heterogeneous networks contain more steady states and a larger *space of possible* than homogeneous networks
- Bifurcation diagrams reveal that large systems contain a “continuum” of steady states
- The case of single and two CSTR is extended to larger 2D systems
- Future work will include stability analysis and dynamic bifurcation diagrams

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