An Agent-Based Framework for Control of Reactor Networks with Autocatalytic Replicators

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Outline

I. Complex systems

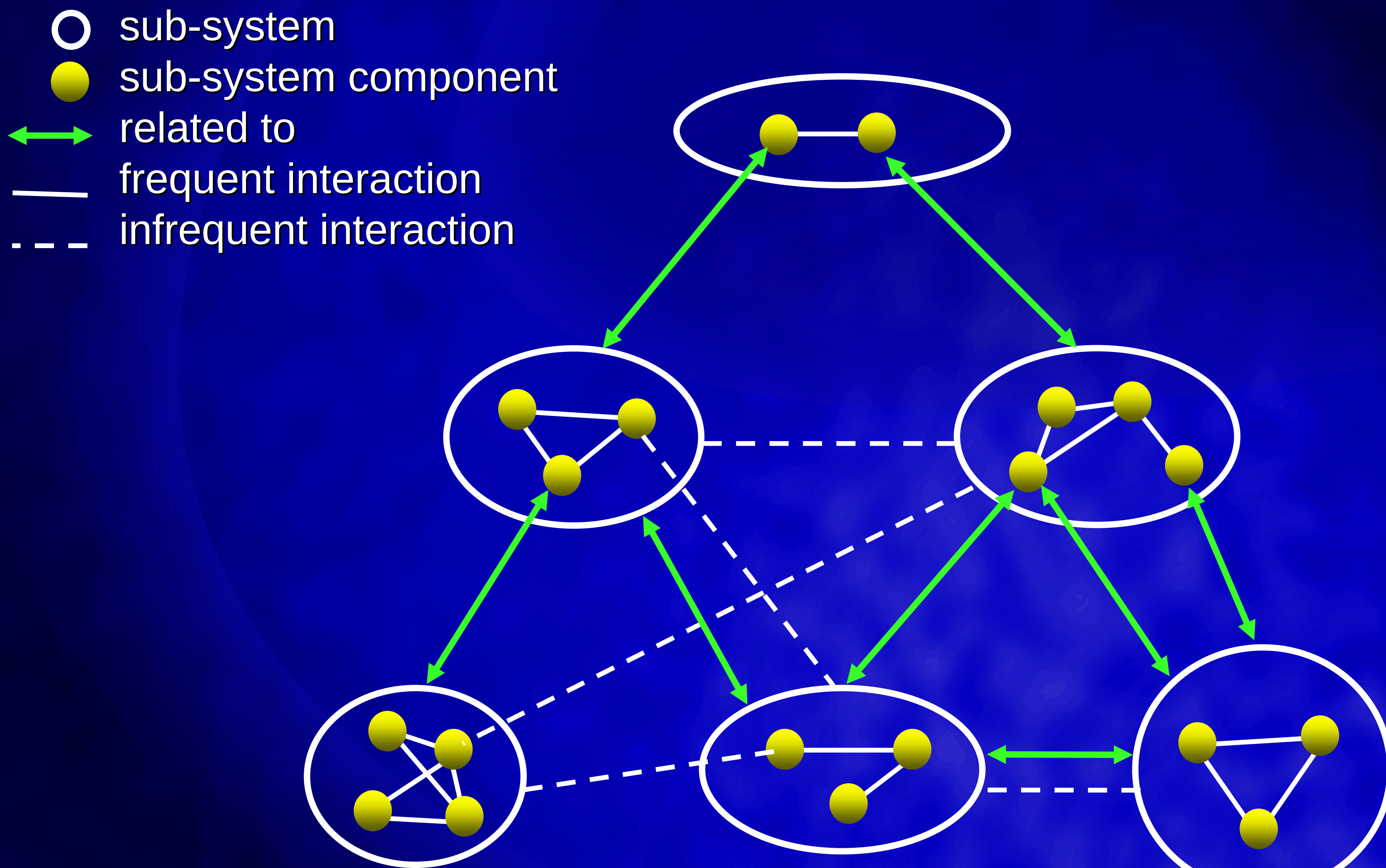
II. Agent-based systems

III. Reactor networks – statics, dynamics

IV. Agent control scheme

V. Case studies

Canonical View of a Complex System



(Jennings and Bussmann, 2003)

Control of Complex Systems

Observing, managing, and controlling complex systems is difficult

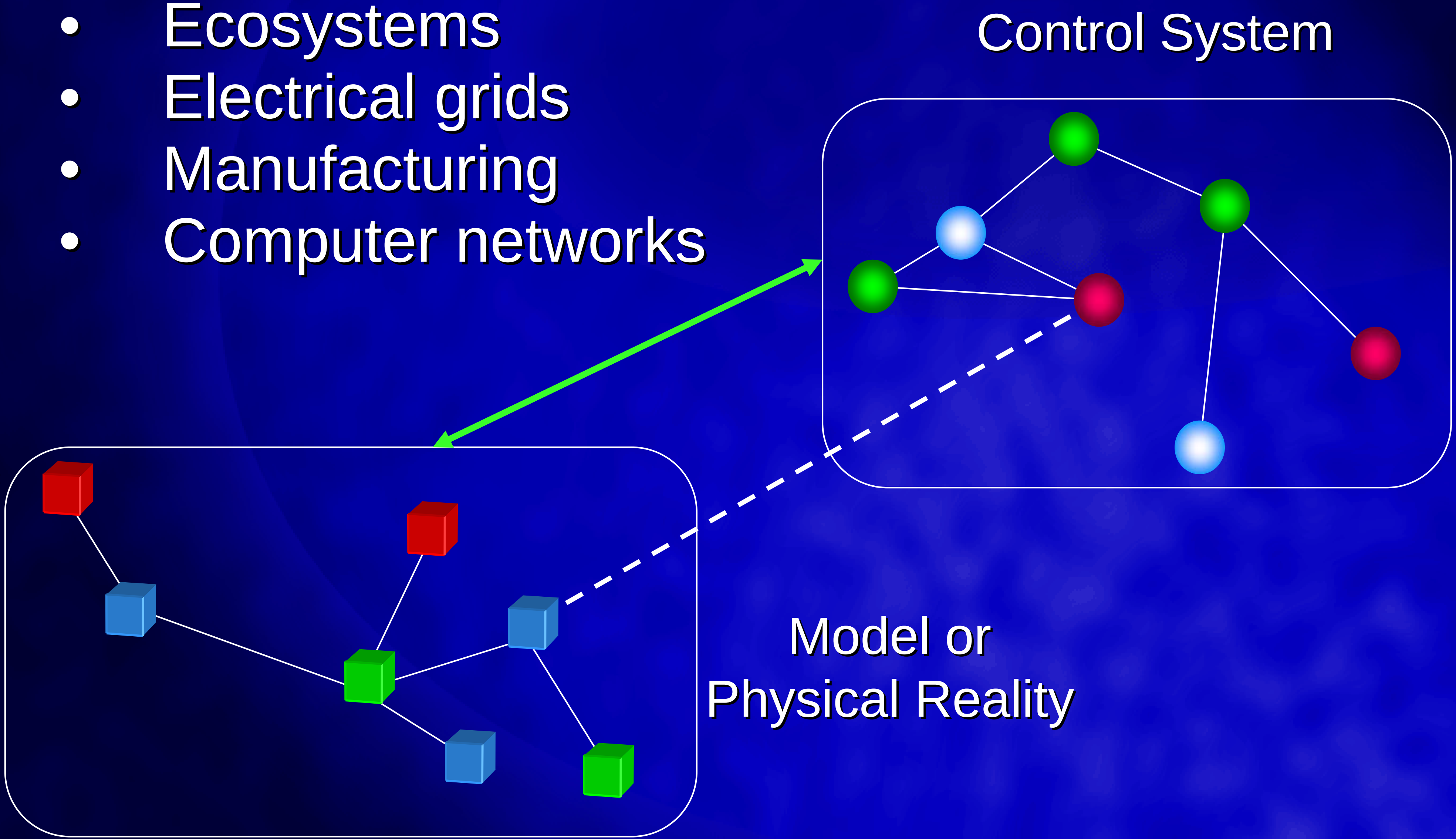
- Large number of variables to monitor
- Unpredictable system behavior
- Multi-stability
- Multiple control strategies

Traditional nonlinear control schemes

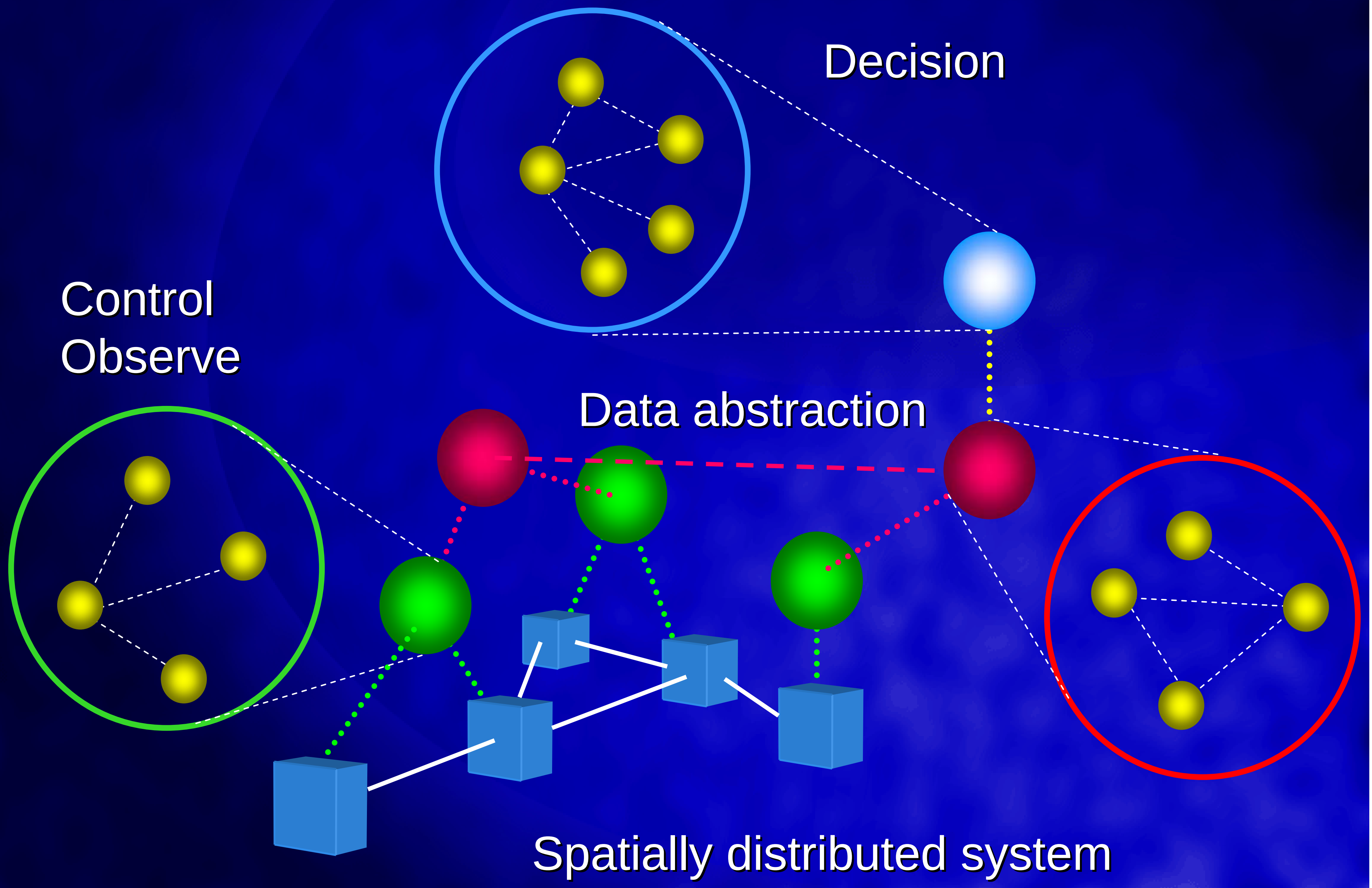
- Model reduction
- A priori determined actuator configurations

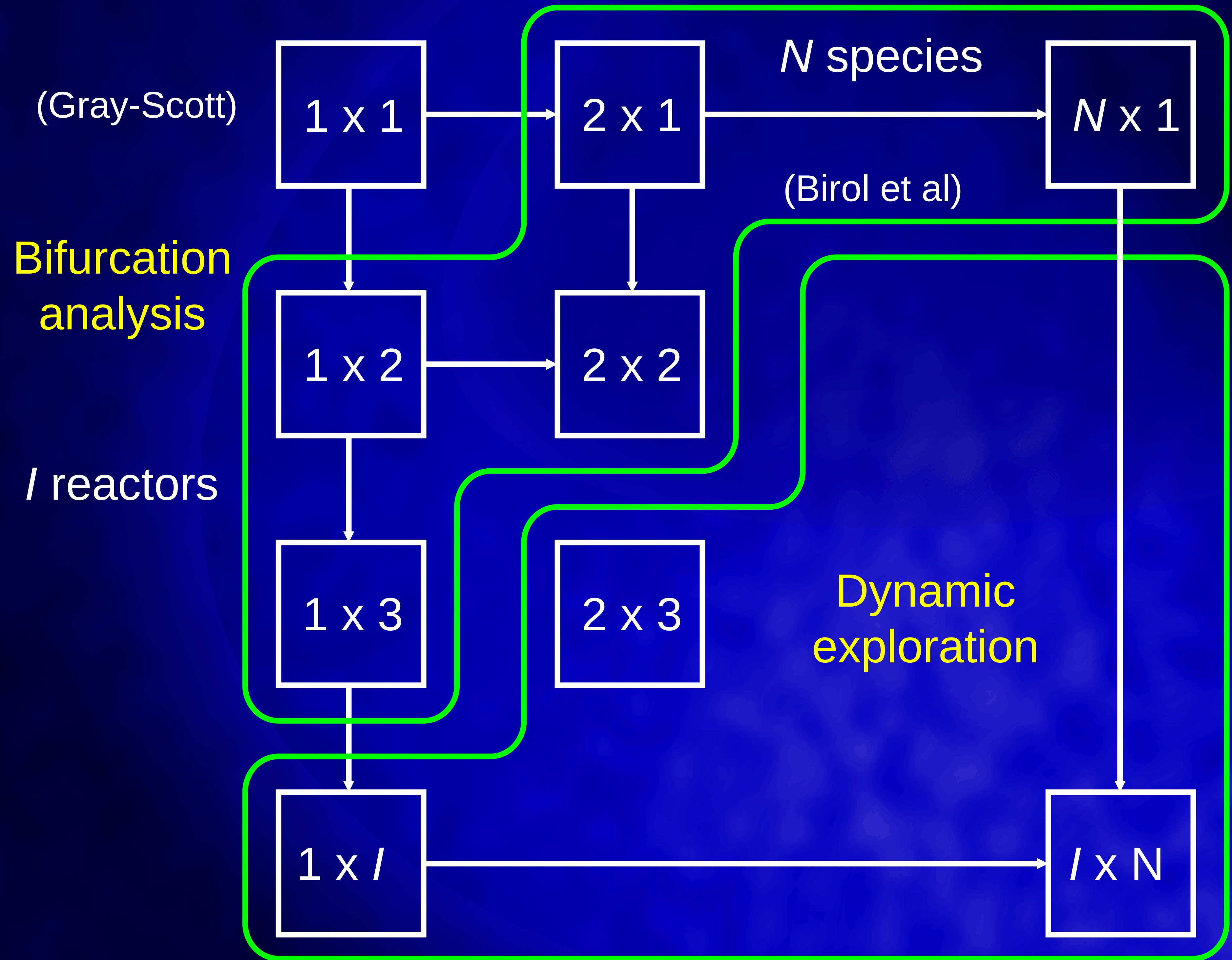
Agent Models + Monitoring

- Financial Markets
- Ecosystems
- Electrical grids
- Manufacturing
- Computer networks



Agent-Based Monitoring / Control




(Gray-Scott)
1 x 1
2 x 1
N species
N x 1
(Birol et al)
Bifurcation analysis
1 x 2
2 x 2
I reactors
1 x 3
2 x 3
Dynamic exploration
1 x *I*
I x N

Reactor Network

R	resource concentration
R_0	resource concentration in feed
P_n	species *n* concentration
D	dead species
r_i	R/R_0 in reactor *i*
p_{in}	P/R_0 in reactor *I*
k_n	growth rate of species *n*
d_n	death rate of species *n*
f	feed flow rate
g	interaction flow rate
t	time

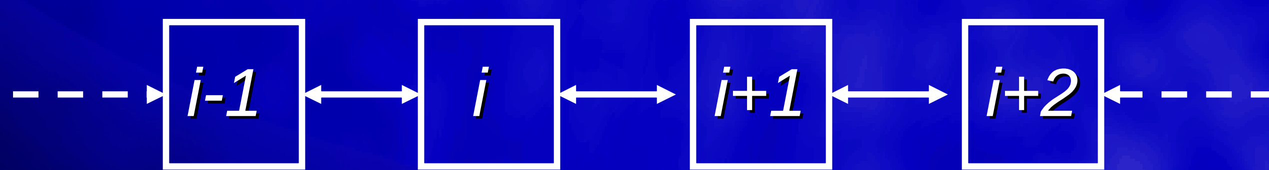
$$R + 2P_n \xrightarrow{k_n} 3P_n$$

$$P_n \xrightarrow{d_n} D$$

$$\frac{dr_i}{dt} = -\sum_{n=1}^{N} k_n r_i p_{in}^2 + f\left(1 - r_i\right) + g\left(r_{i-1} + r_{i+1} - 2r_i\right)$$

net loss to reaction — net loss to in/outflow, death — net loss to neighbors

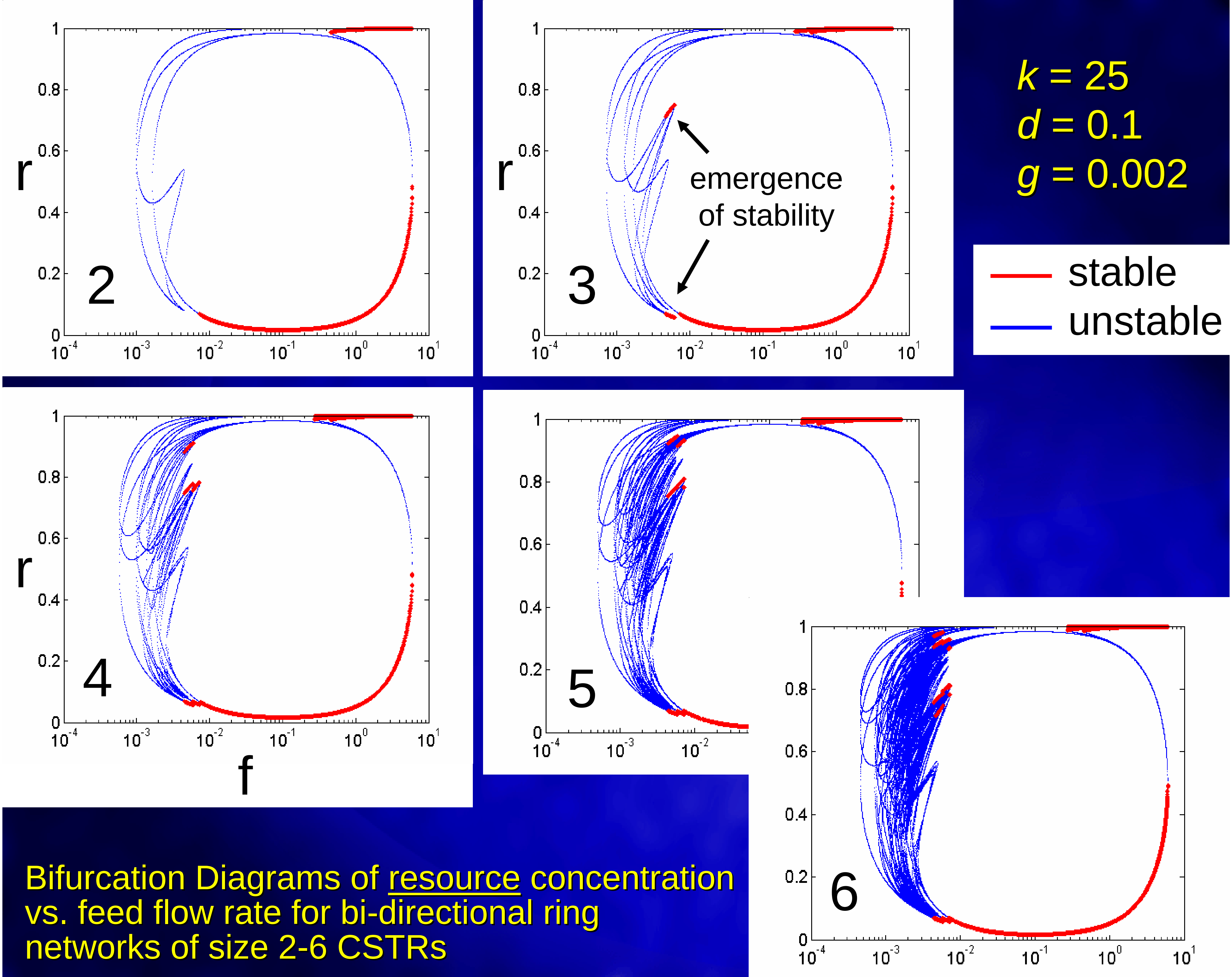
$$\frac{dp_{in}}{dt} = k_n r_i p_{in}^2 - p_{in}\left(f + d_n\right) + g\left(p_{i-1,n} + p_{i+1,n} - 2p_{in}\right)$$



Reactor Networks

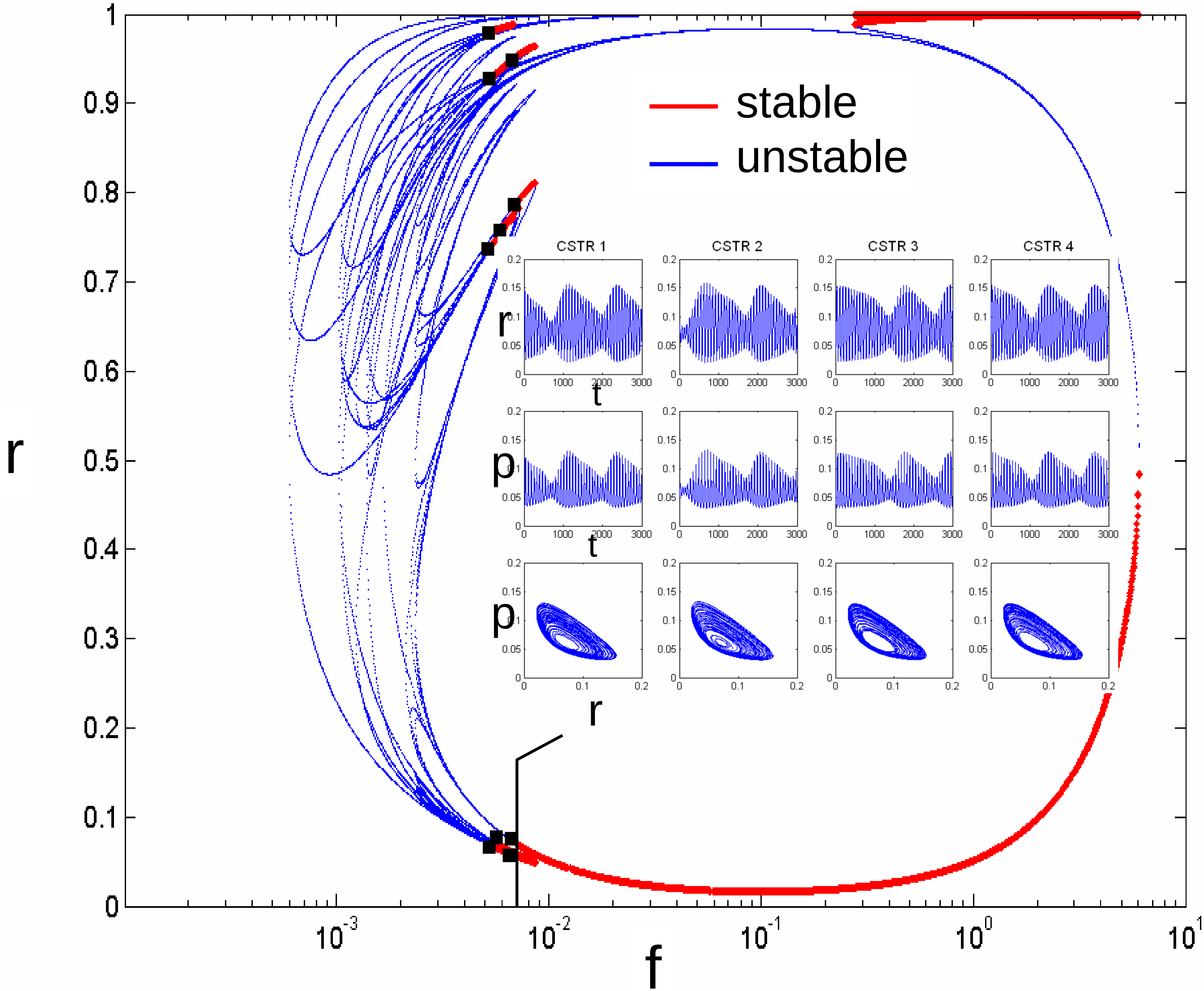
Effects of increased spatial heterogeneity

- Complex behavior
- Steady states increase exponentially
- Coexistence of competitors
- Sustained oscillations
  - Phase locking: strong coupling
  - Quasiperiodicity: weak coupling
  - Traveling waves
- Emergence
  - Enlarge species existence space

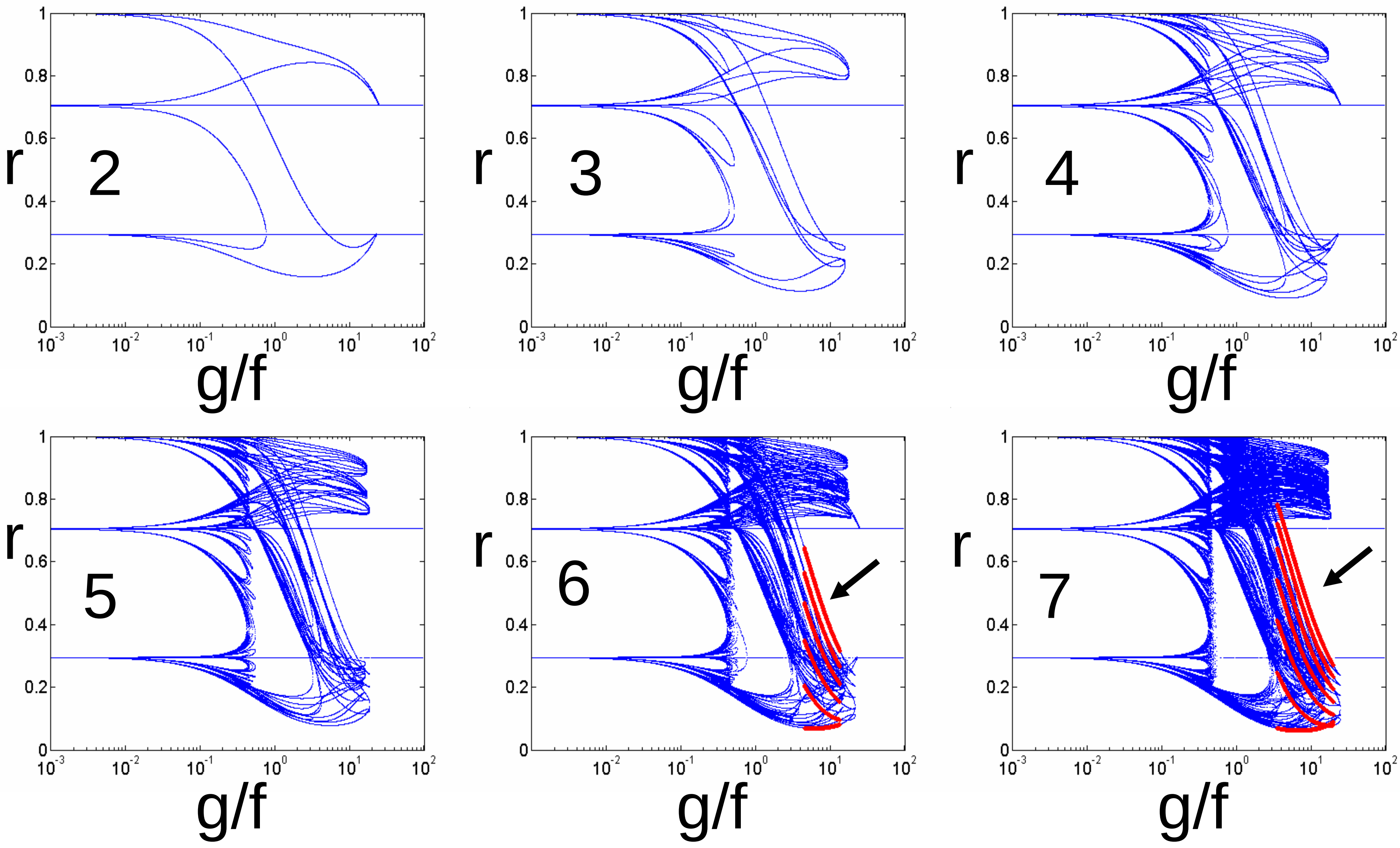


Bifurcation Diagrams of resource concentration vs. feed flow rate for bi-directional ring networks of size 2-6 CSTRs

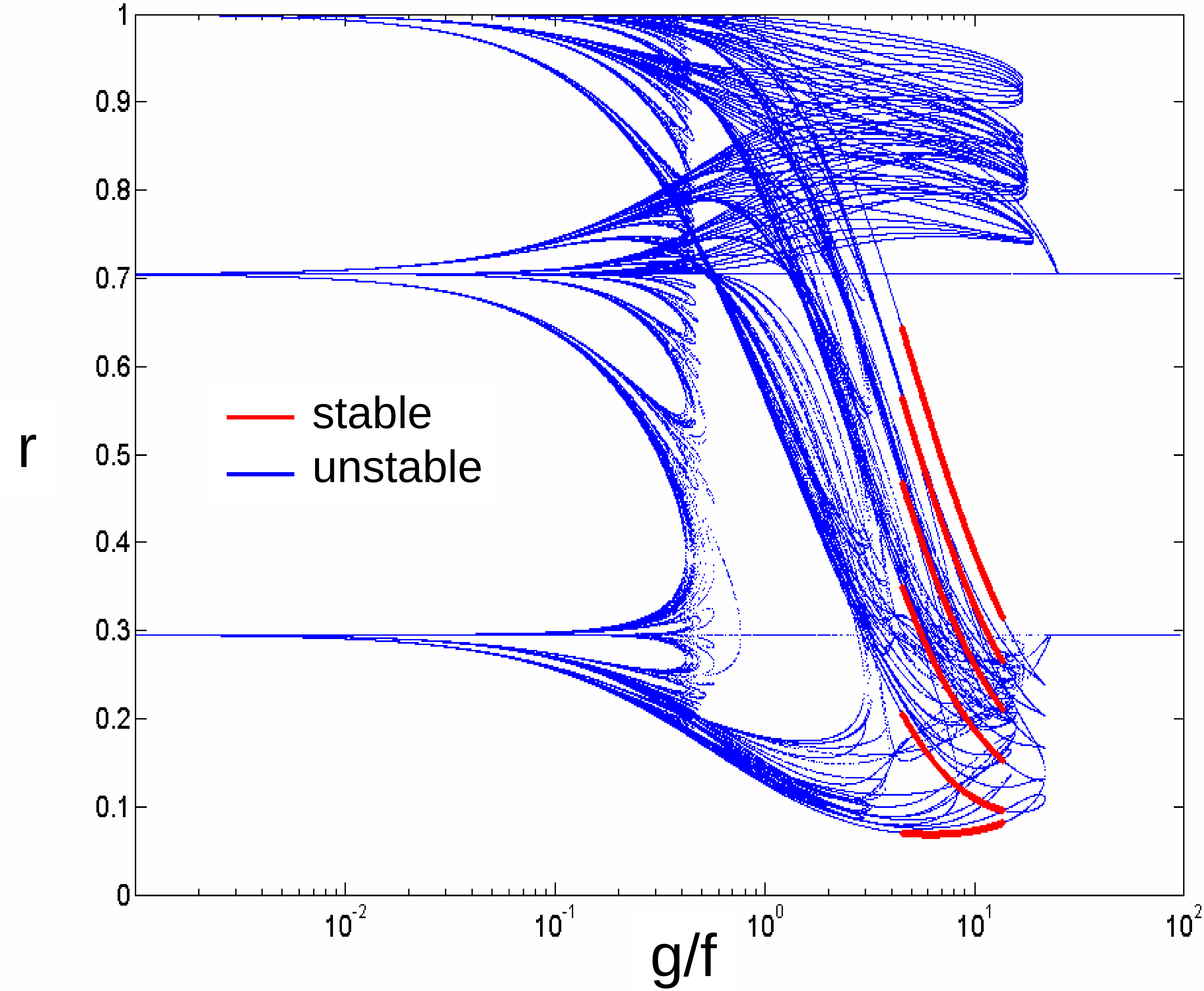
Bifurcation diagram for 4-CSTR uni-directional ring network



Bifurcation Diagrams of resource concentration vs. interconnection flow rate / feed flow rate (*g* / *f*) for uni-directional ring networks of size 2-7 CSTRs



Bifurcation diagram for 6-CSTR uni-directional ring network

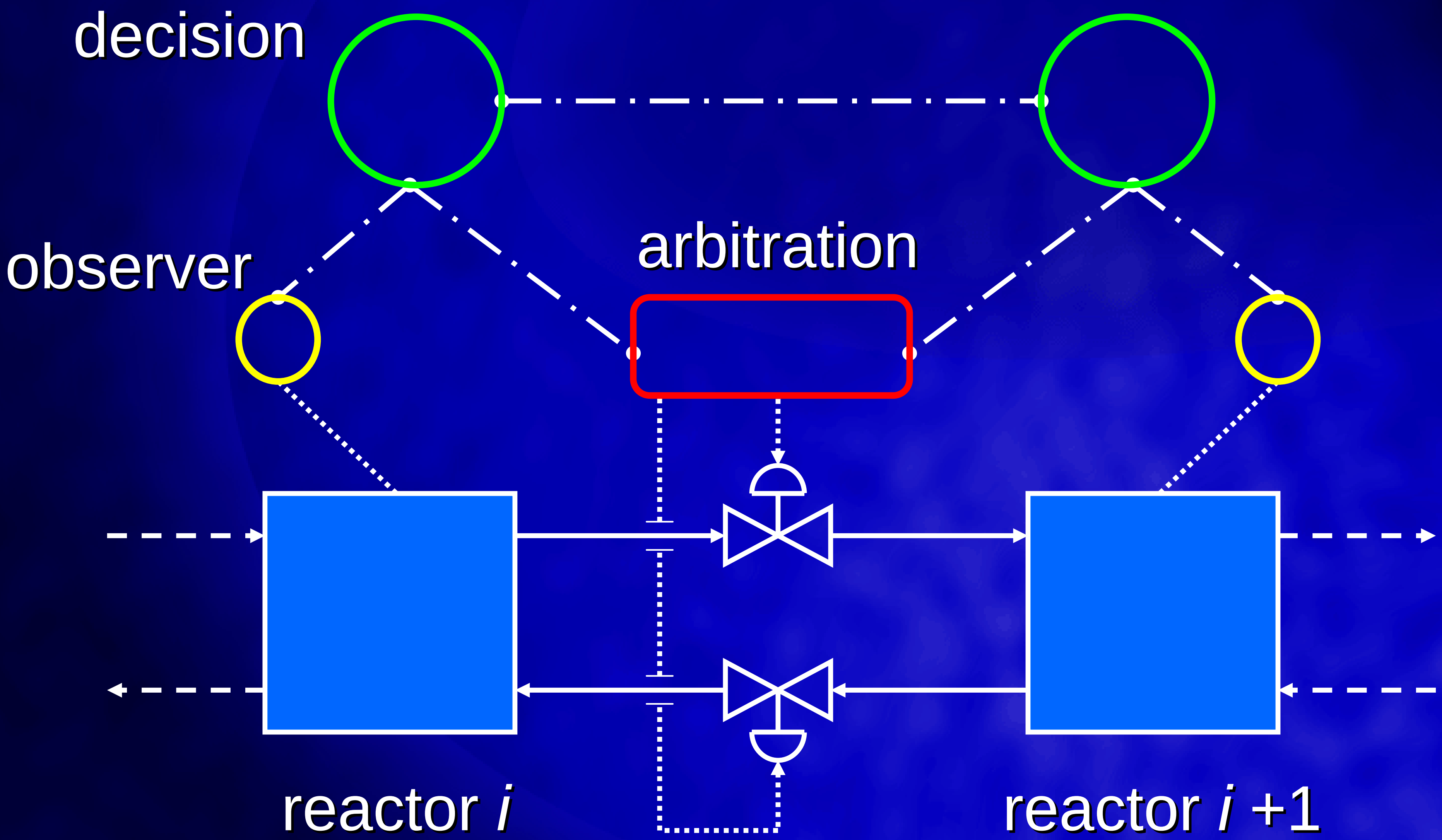


Reactor Networks – Control

- Nonlinear control scheme : species conc.
  1. Remove undesirable species
  2. Populate desirable species
  3. Transients through several operating regimes
- Multiple controllers needed
- Combinations of local control objectives

➡ Hierarchical control structure

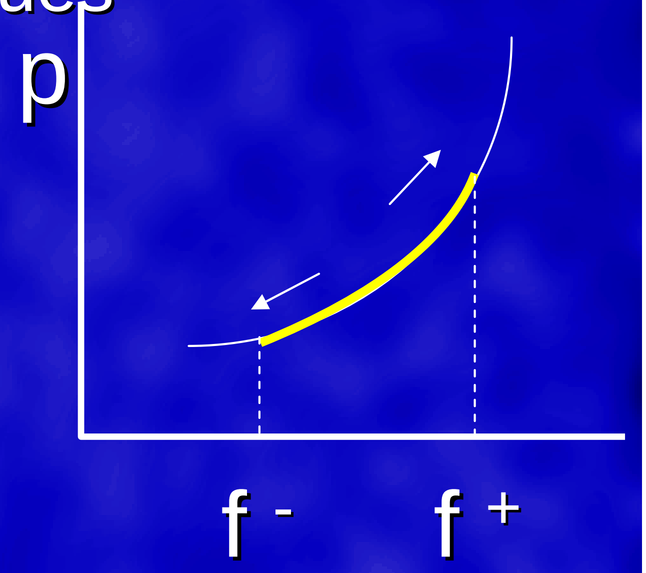
Agent Control Scheme



Agent Control Scheme

- Each agent has some level of control over the interaction of its neighbors
- Arbitrator receives operational requests from other agents
- Agents set max / min compromise values
- Agents may cooperate or compete
- Extinction is to be avoided at all costs

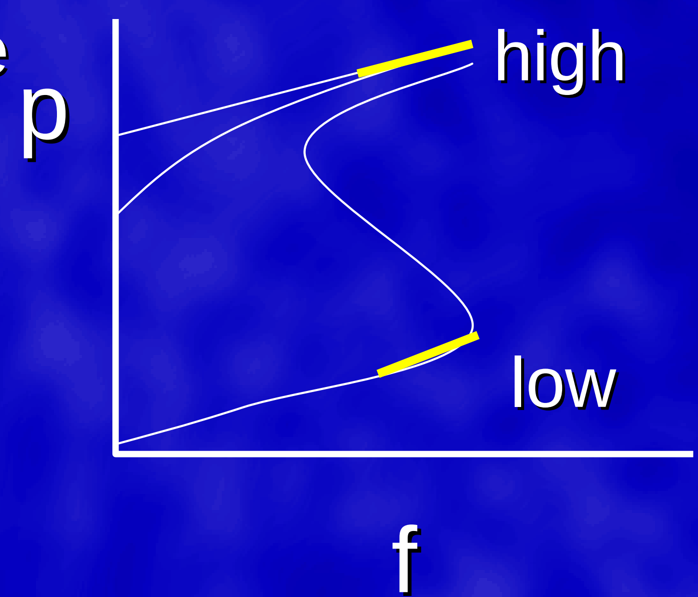
  by avoiding unstable regions



Agent Control Scheme

- A reactor may operate at one of many multiple states
- Agents try to improve operating conditions
  - Increase species concentration
  - Request assistance from neighbors
- Disadvantaged agent may negotiate

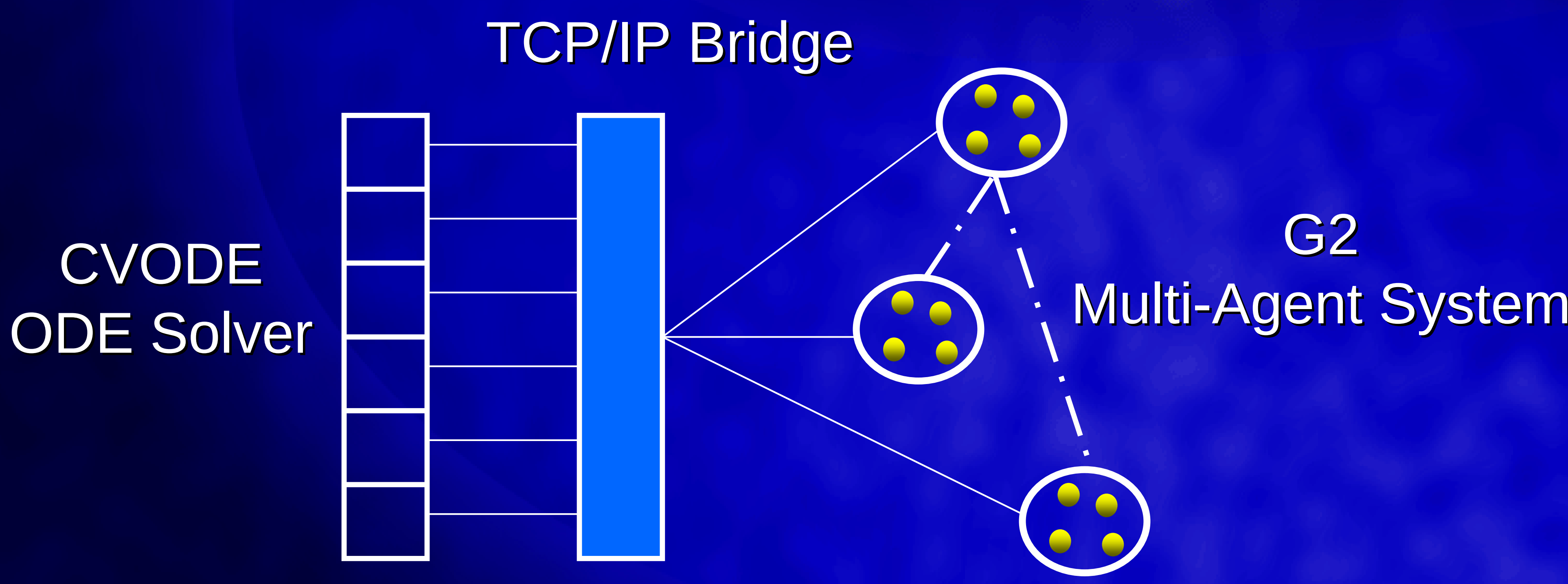
  for a more favorable outcome

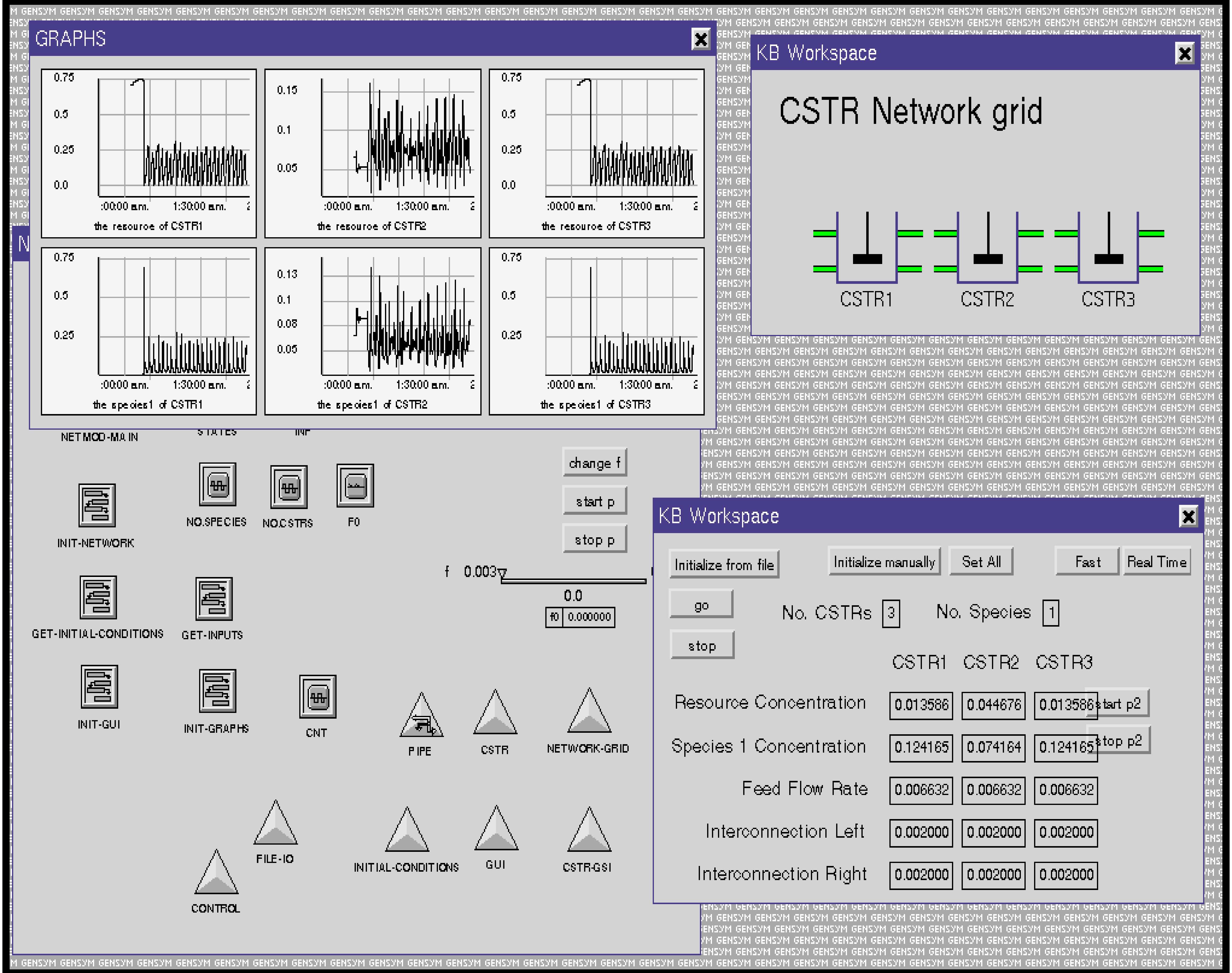


Software Tools

- Gensym G2
- CVODE libraries

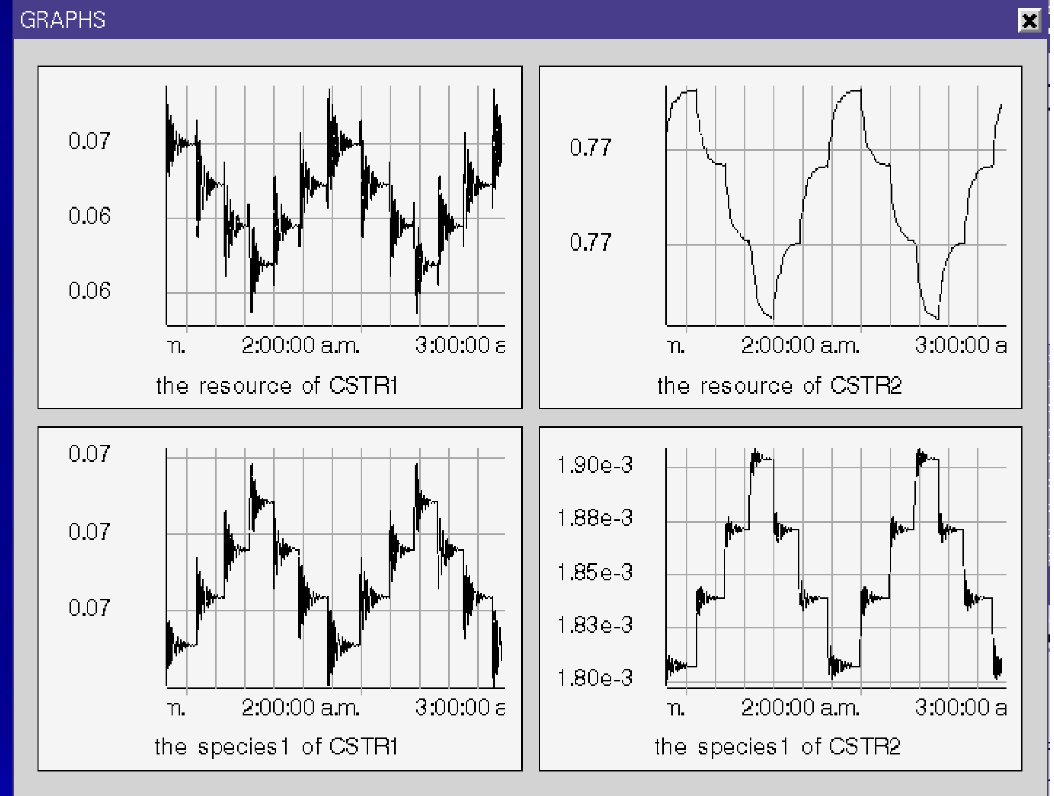
- KBS development shell
- Graphical interface
- Object oriented language
- real-time intelligent applications

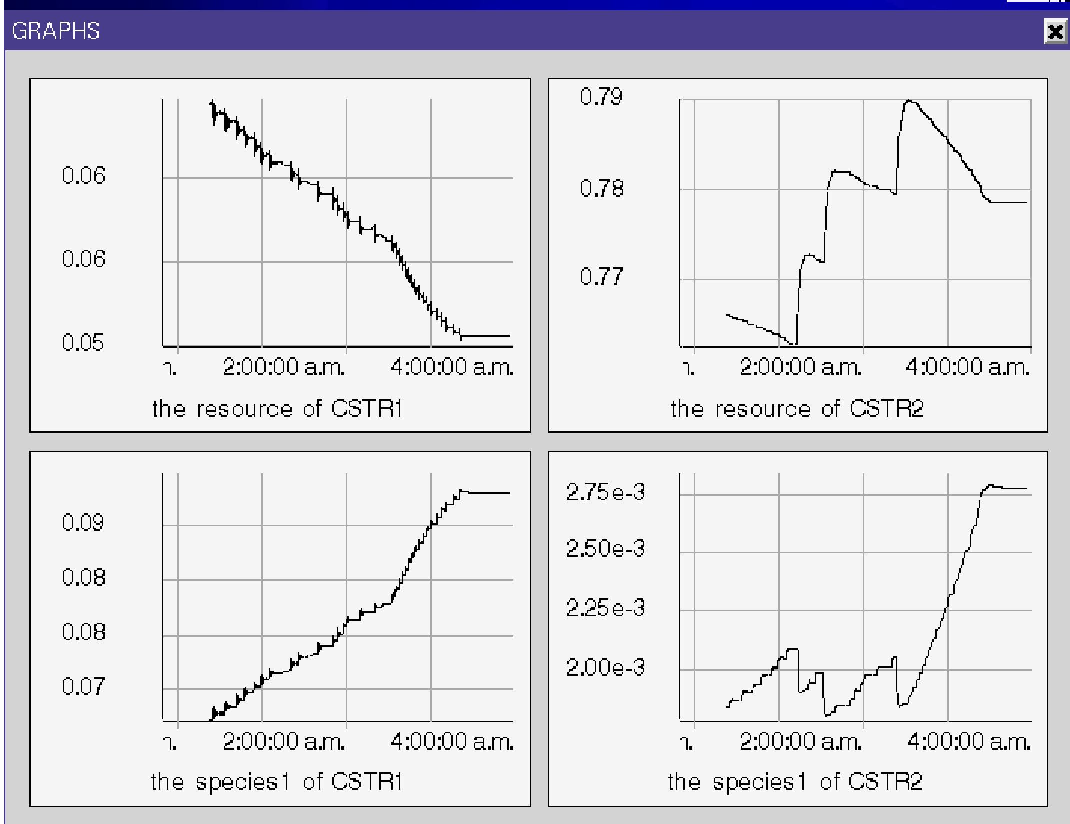



GRAPHS
the resource of CSTR1
the resource of CSTR2
the resource of CSTR3
the species1 of CSTR1
the species1 of CSTR2
the species1 of CSTR3
KB Workspace
CSTR Network grid
CSTR1
CSTR2
CSTR3
NETMOD-MAIN
NO.SPECIES
NO.CSTRS
F0
INIT-NETWORK
GET-INITIAL-CONDITIONS
GET-INPUTS
INIT-GUI
INIT-GRAPHS
CNT
PIPE
CSTR
NETWORK-GRID
FILE-IO
INITIAL-CONDITIONS
GUI
CSTR-GSI
CONTROL
change f
start p
stop p
f 0.003
0.0
f0 0.000000
KB Workspace
Initialize from file
Initialize manually
Set All
Fast
Real Time
go
stop
No. CSTRs 3
No. Species 1
CSTR1 CSTR2 CSTR3
Resource Concentration 0.013586 0.044676 0.013586
Species 1 Concentration 0.124165 0.074164 0.124165
Feed Flow Rate 0.006632 0.006632 0.006632
Interconnection Left 0.002000 0.002000 0.002000
Interconnection Right 0.002000 0.002000 0.002000
start p2
stop p2

Case – Local Interactions

Immediate retribution results in oscillation whenever one agent loses.

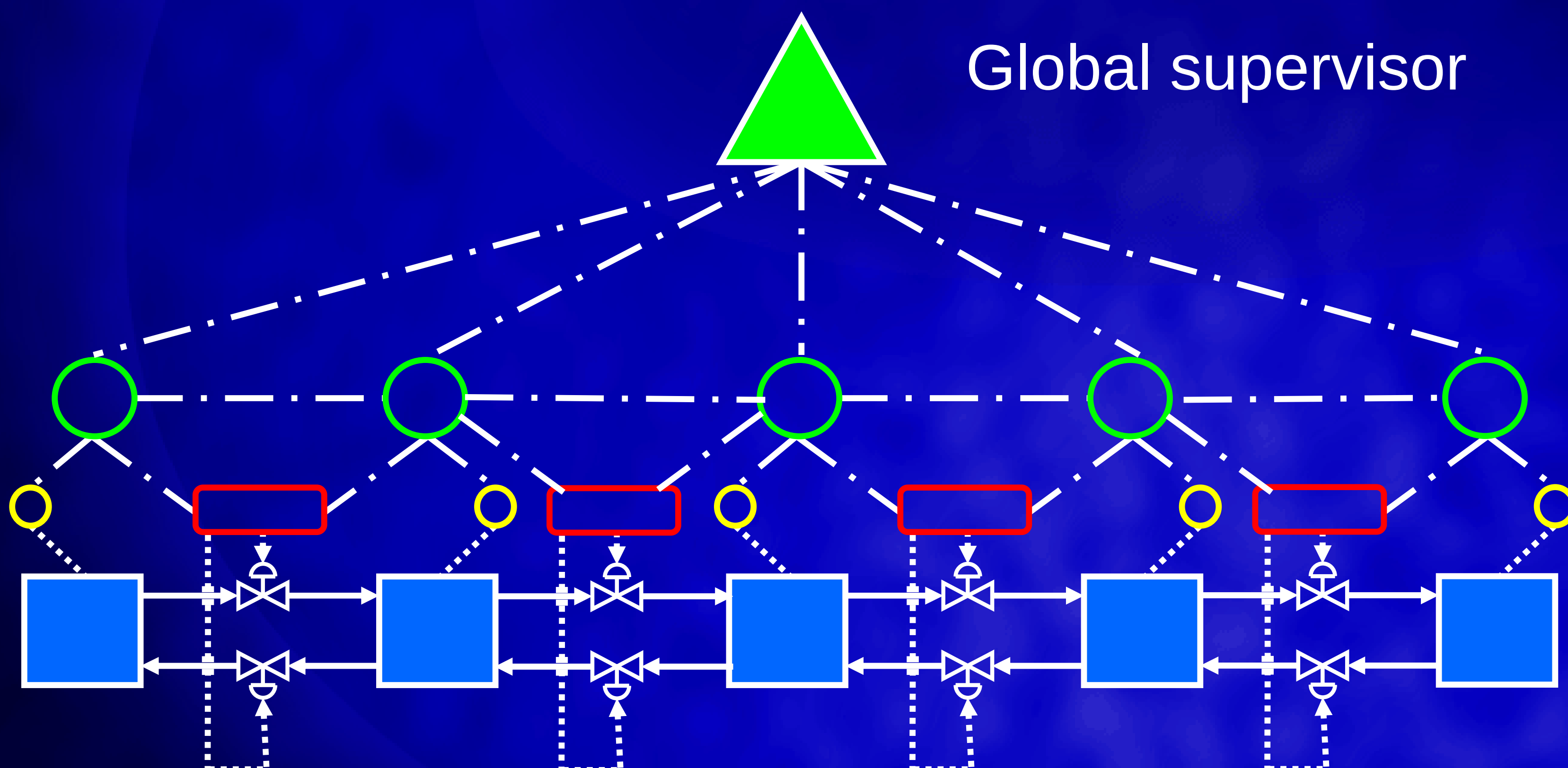




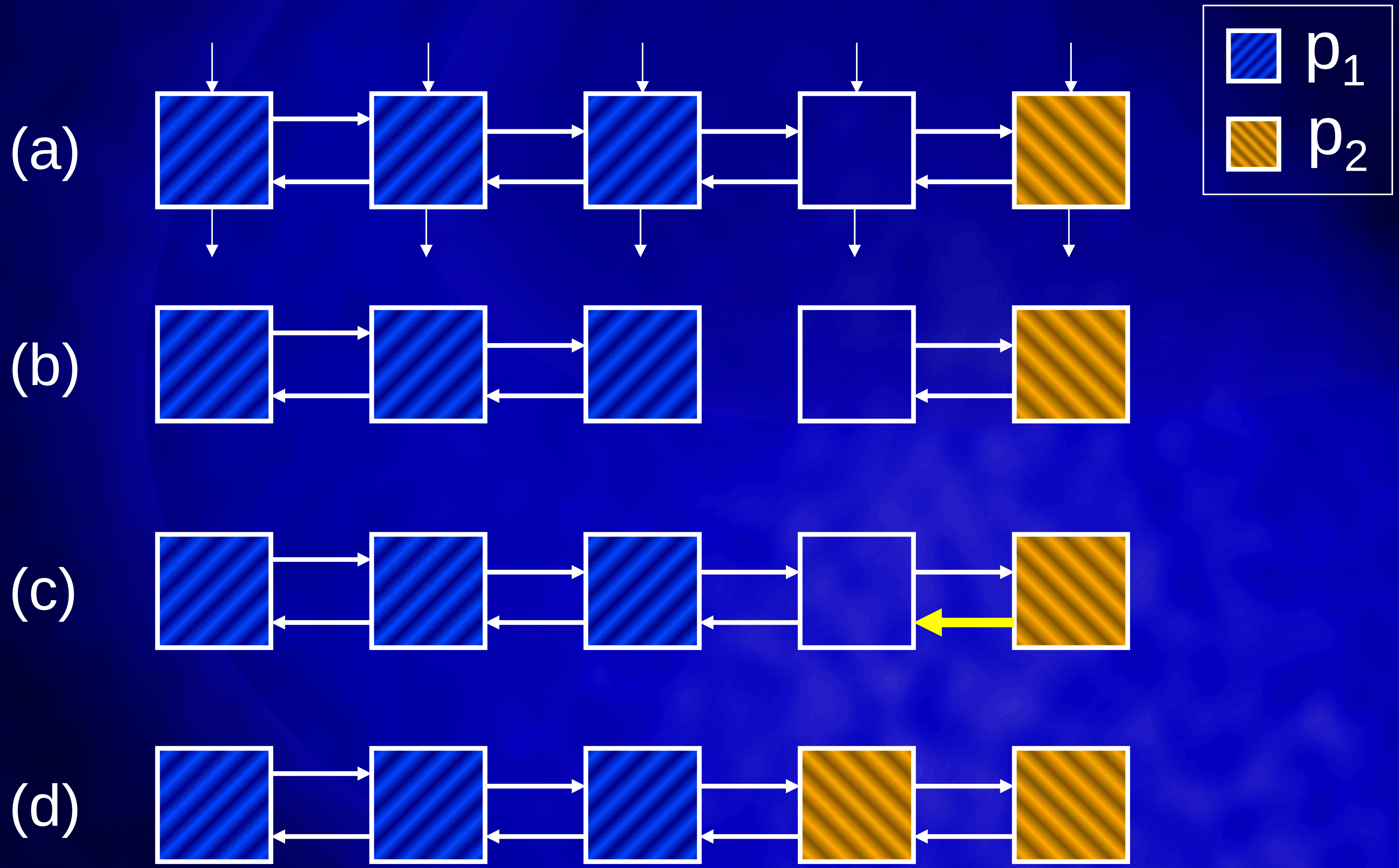
Allowing one loss per turn results in both agents increasing goals incrementally.

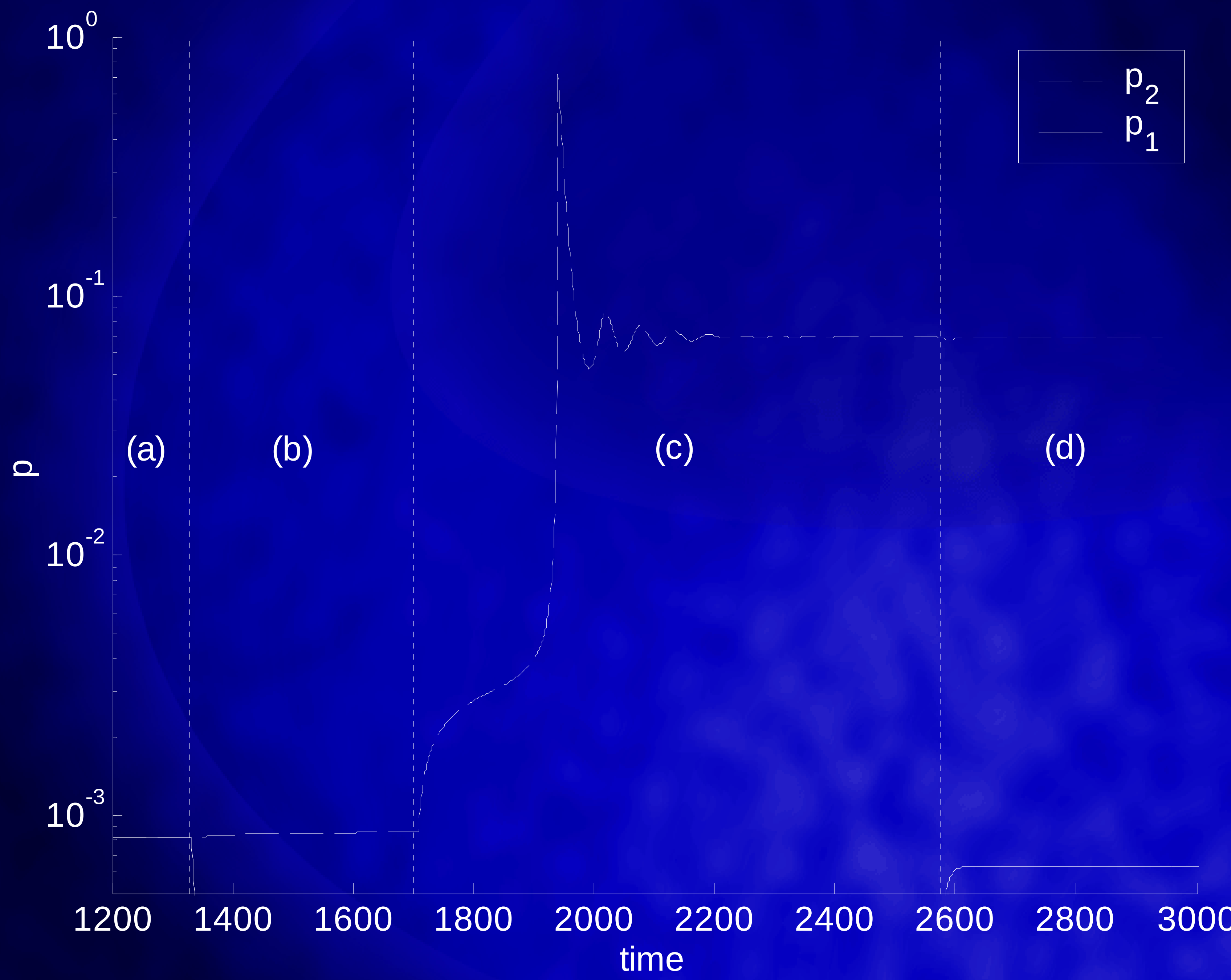
Cases - Global Interactions

Reactor network - alternative hybrid control approach



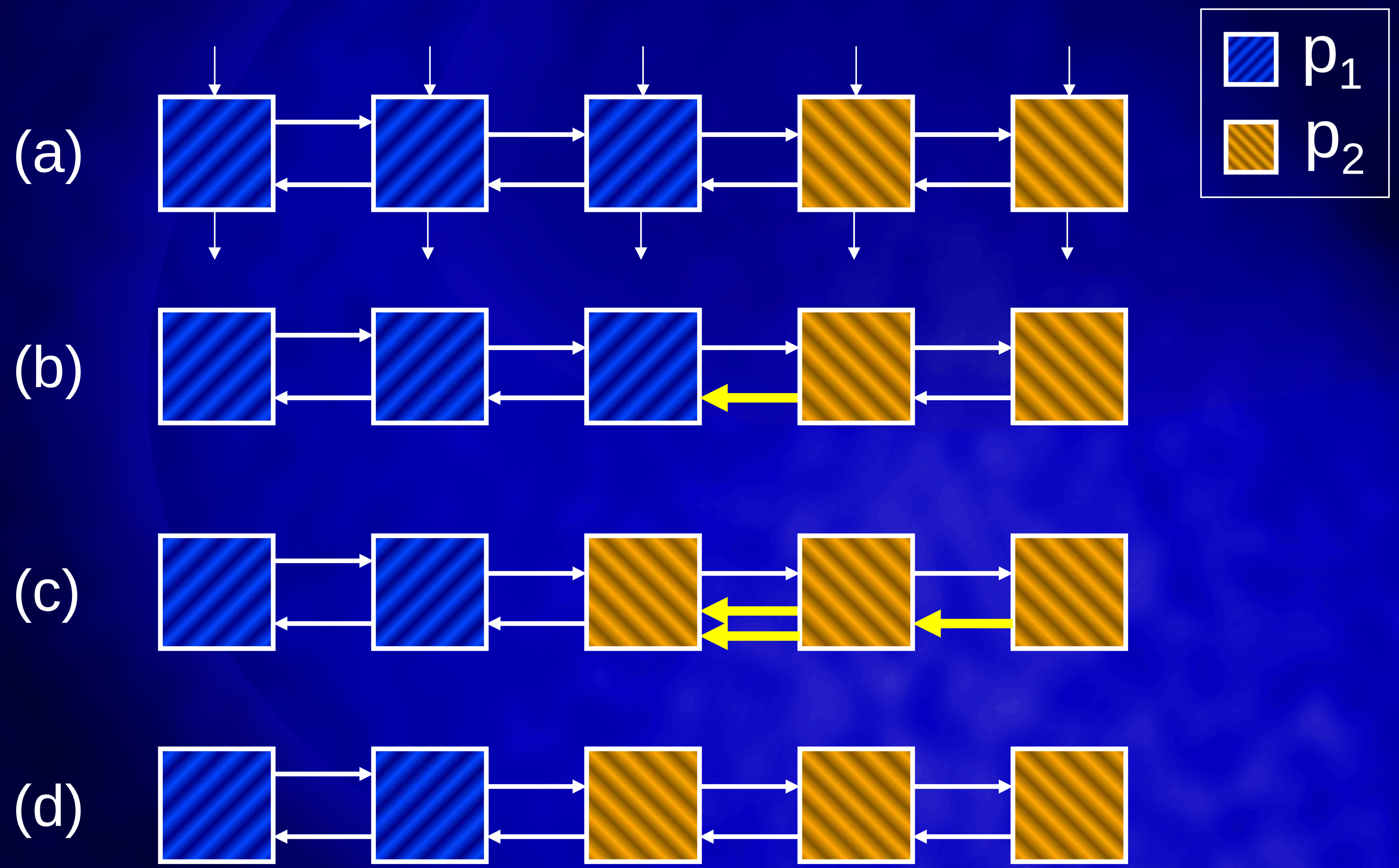
Case 1 – Filling an empty reactor

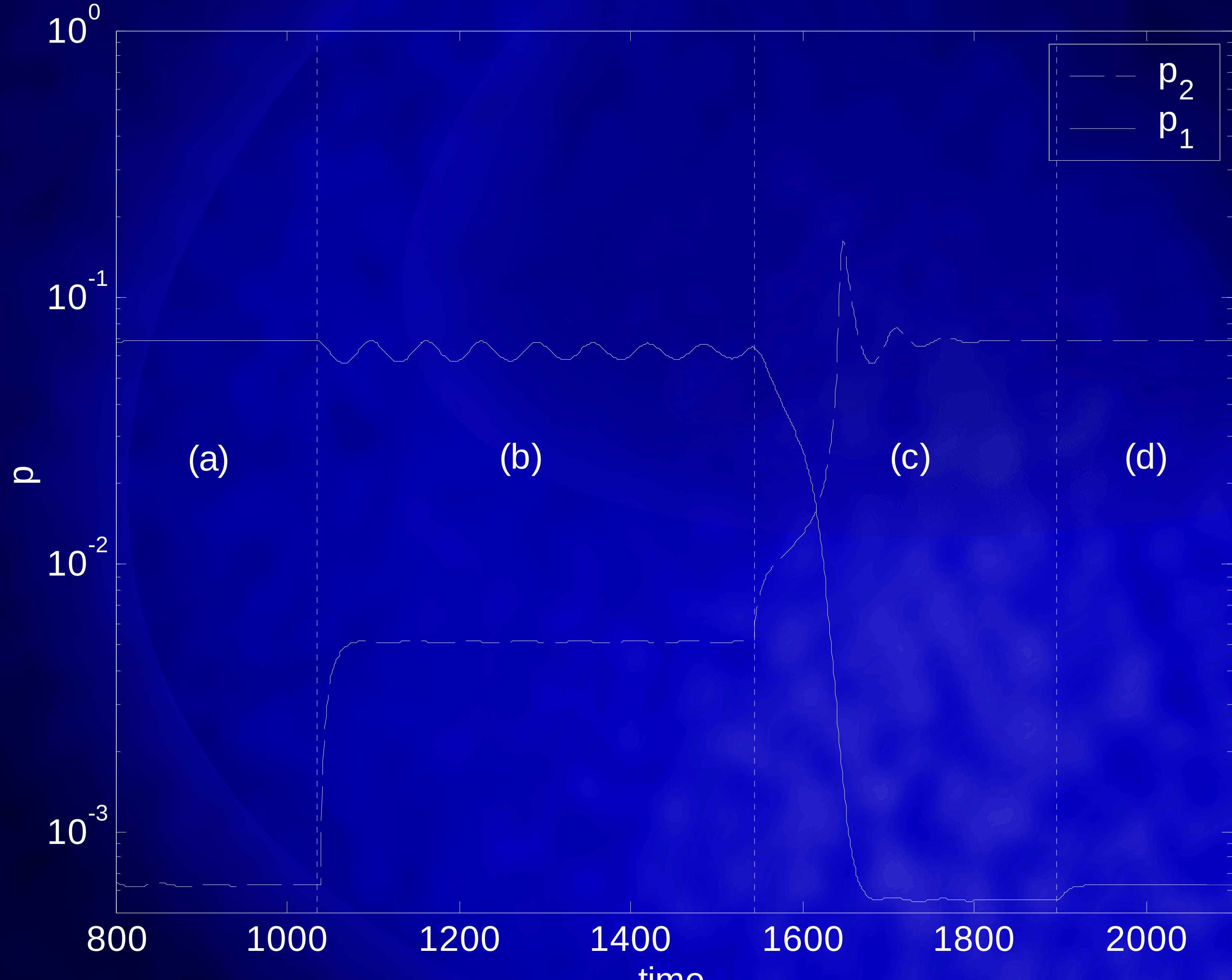




10^0
10^{-1}
10^{-2}
10^{-3}
p
1200
1400
1600
1800
2000
2200
2400
2600
2800
3000
time
(a)
(b)
(c)
(d)
p_2
p_1

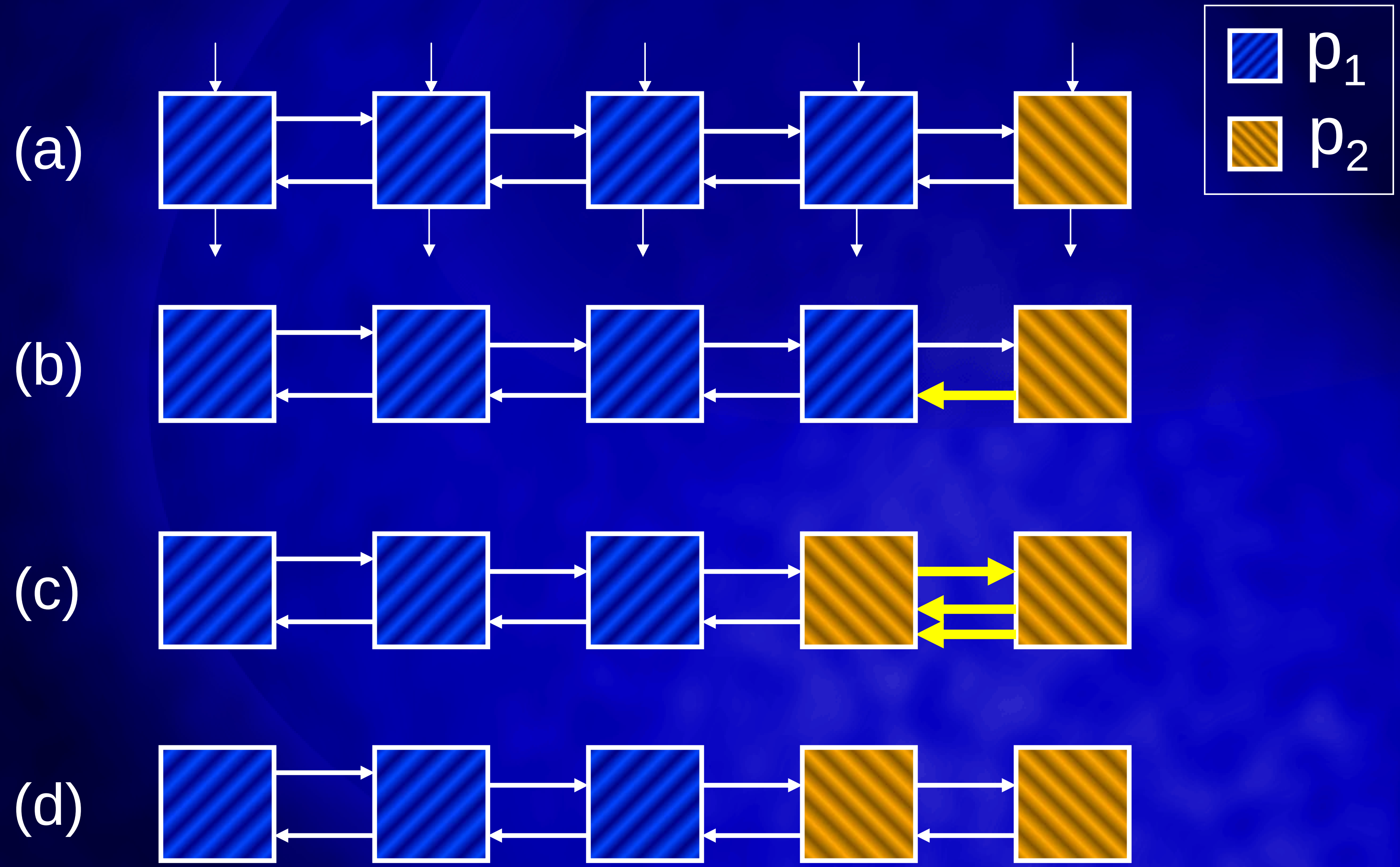
Case 2 – Filling an occupied reactor

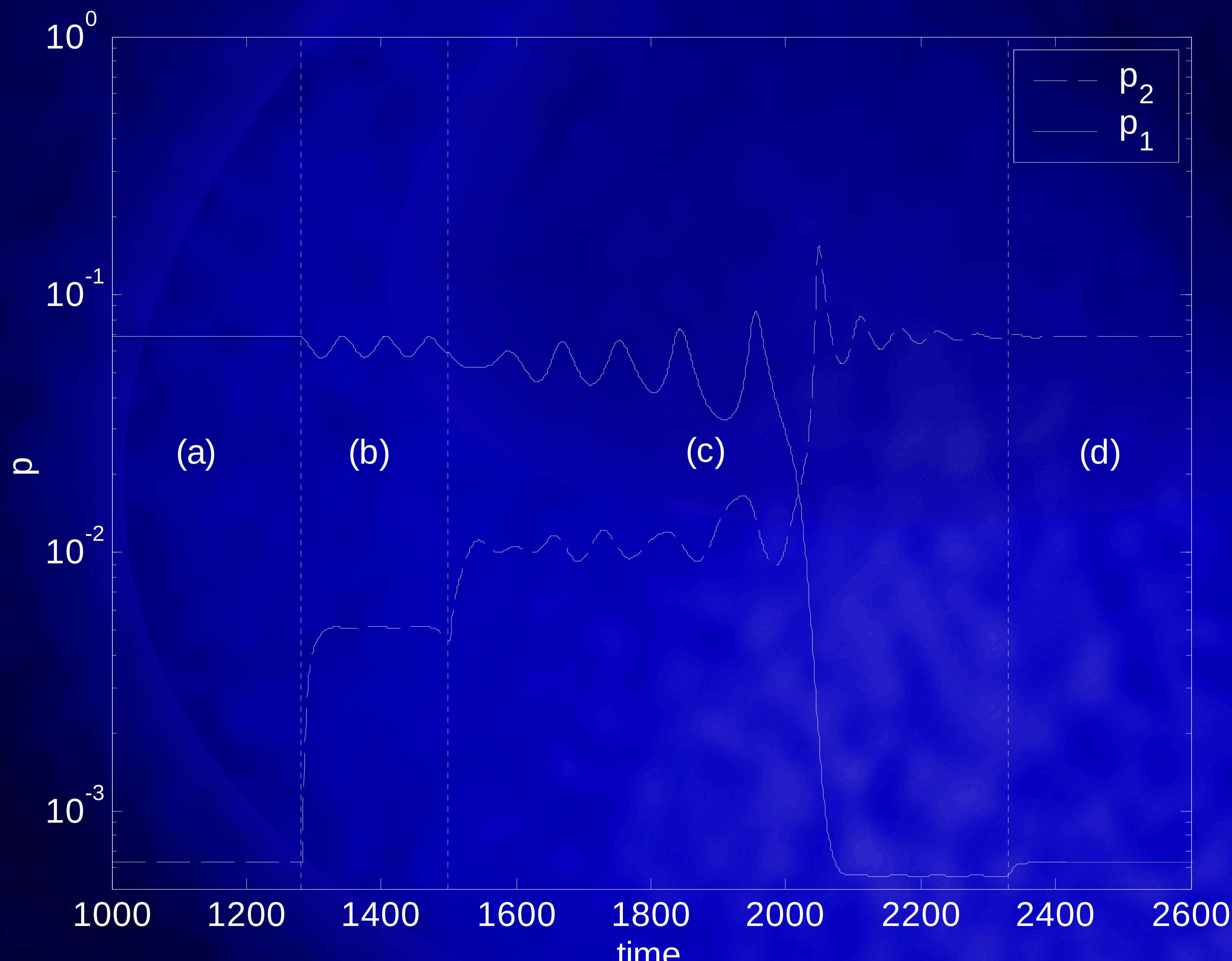




10^0
10^{-1}
10^{-2}
10^{-3}
p
800
1000
1200
1400
1600
1800
2000
time
(a)
(b)
(c)
(d)
p_2
p_1

Case 3 – Filling an occupied reactor II





10^0
10^{-1}
10^{-2}
10^{-3}
p
(a)
(b)
(c)
(d)
p_2
p_1
1000
1200
1400
1600
1800
2000
2200
2400
2600
time

Conclusions

A hybrid multi-layer agent-based system was developed as an alternative to conventional approaches for monitoring and control of spatially distributed processes.

The intelligent agent-based control system successfully controls the spatial distribution of autocatalytic species in a network of reactors.

Contact and Acknowledgments

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