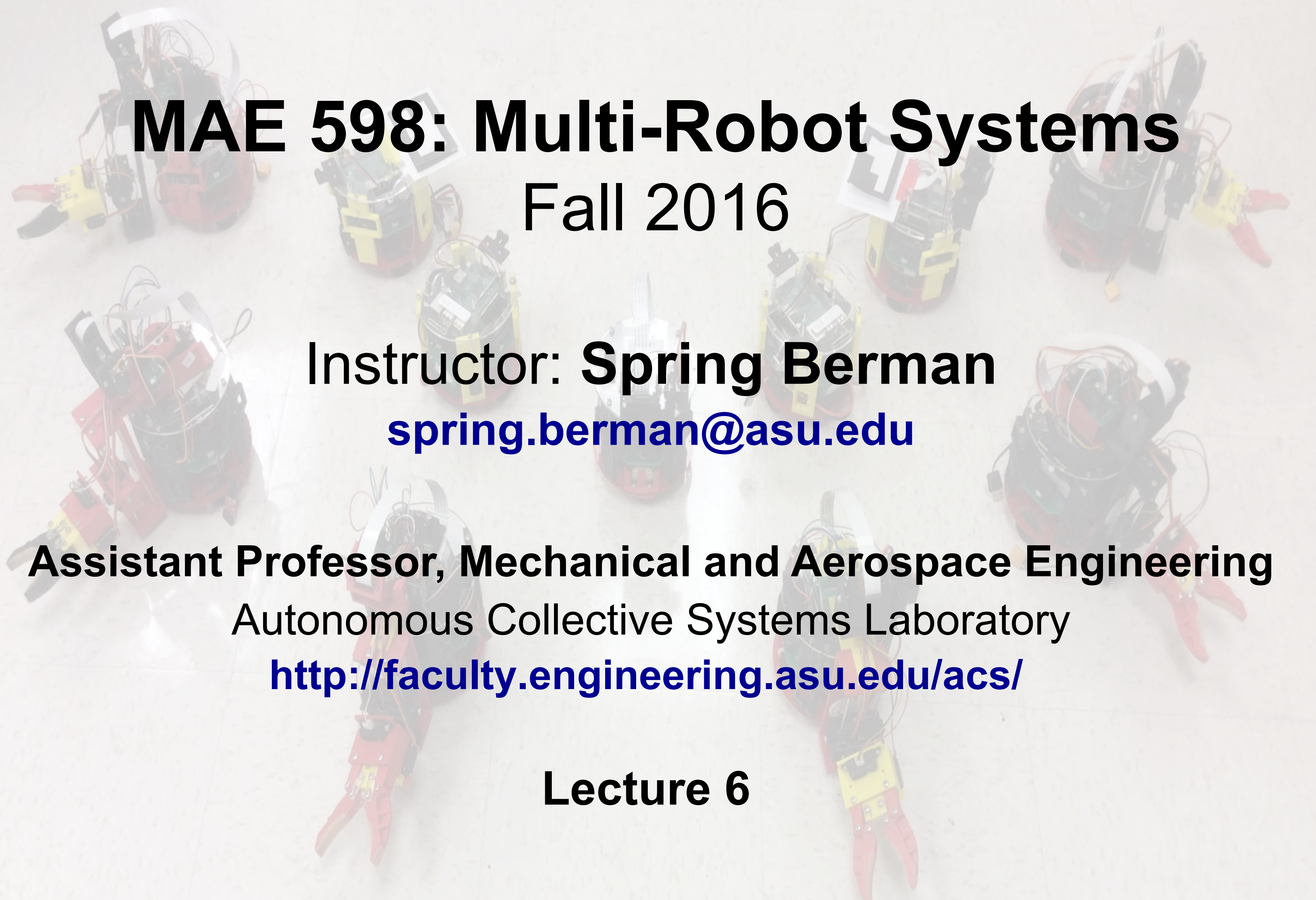

MAE 598: Multi-Robot Systems

Fall 2016

Instructor: **Spring Berman**

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http://faculty.engineering.asu.edu/acs/

Lecture 6

Classifying Dynamical Behavior of Chemical Reaction Networks

Spring Berman

Motivation

- Analysis

Understand cell functions at the level of chemical interactions [Angeli, de Leenheer, Sontag, *CDC 2006*]

- functionality, qualitative behavior of pathways
- robustness of network to parameter changes

- Synthesis

Determine whether a network will produce the desired behavior, or at least have the capacity to produce it

- drug design, therapeutic treatments
- bio-inspired distributed robot systems

Approaches

- There is presently no unified theory of the dynamical behavior of chemical reactions
  [De Leenheer, Angeli, Sontag, *J. Math. Chem.* 41:3, April 2007]

- However, there are results for restricted classes of reaction networks:
  - Feinberg, Horn, Jackson

    Fairly general network topology, mass-action kinetics

  - Angeli, de Leenheer, Sontag

    Restricted network topology, monotone but otherwise arbitrary kinetics

Feinberg, Horn, Jackson

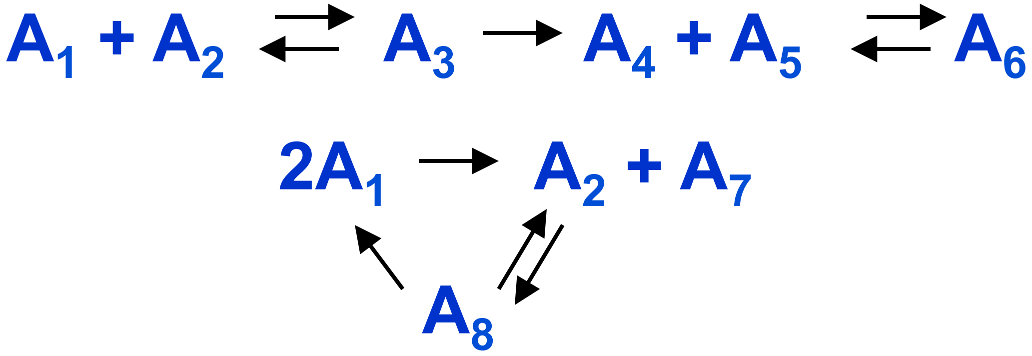
Deficiency Zero and Deficiency One Theorems

Martin Feinberg. Chemical reaction network structure and the stability of complex isothermal reactors – I. The Deficiency Zero and Deficiency One Theorems. *Chem. Eng. Sci.* 42:10 pp. 2229-2268, 1987.

For related publications, see:

http://www.che.eng.ohio-state.edu/~FEINBERG/PUBLICATIONS/

Notation



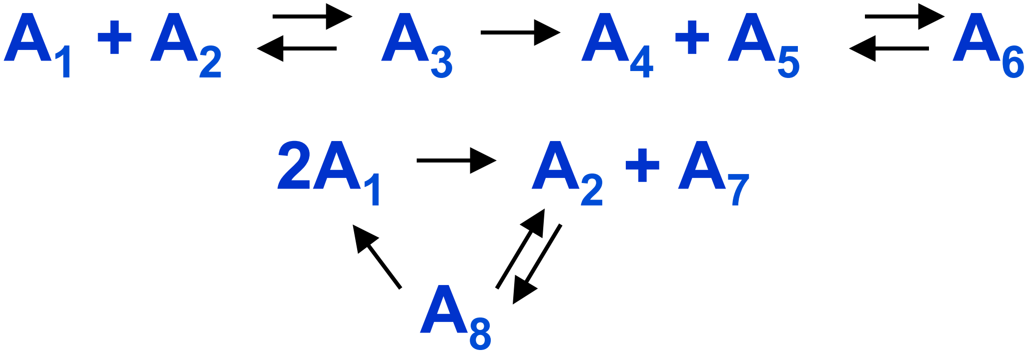
$A_1 + A_2 \rightleftarrows A_3 \rightarrow A_4 + A_5 \rightleftarrows A_6$

$2A_1 \rightarrow A_2 + A_7$

A_8

	Symbol	Example above
Number of species	N	**8**
Number of complexes	n	**7**
Complex vector	$y_i \in \mathbf{R}^N$	$y_1 = [1\ 1\ 0\ 0\ 0\ 0\ 0\ 0]$
Reaction vector	For $y_i \rightarrow y_j$: $y_j - y_i$	$y_2 - y_1 = [-1\ -1\ 1\ 0\ 0\ 0\ 0\ 0]$
Network rank	s	**5**
[# of elements in largest linearly independent set of reaction vectors]		
Number of linkage classes	l	**2**
[set of complexes connected by reactions]		

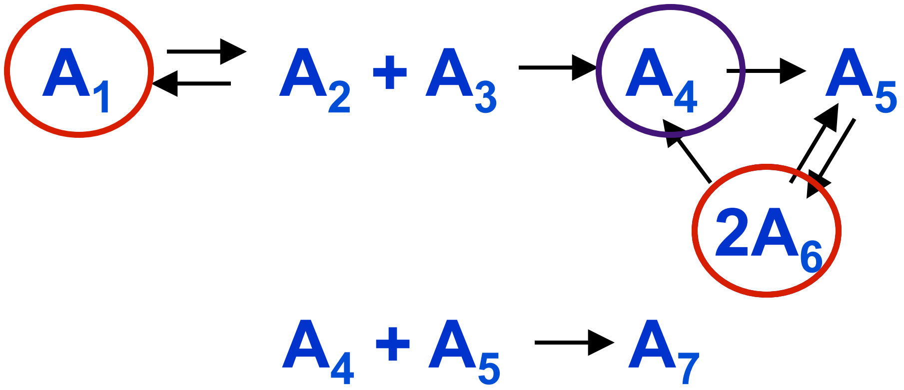
Notation



	Symbol	Example above
Number of complexes	n	7
Network rank	s	5
[# of elements in largest linearly independent set of reaction vectors]		
Number of linkage classes	l	2
[set of complexes connected by reactions]		
Deficiency	$\delta = n - l - s$	0

Definitions

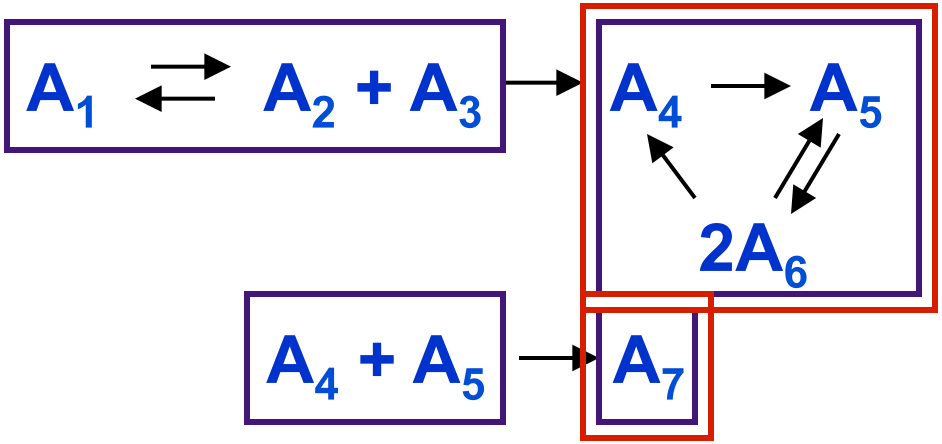
- Reversible: Each reaction is accompanied by its reverse
- Weakly reversible: When there is a directed arrow pathway from complex 1 to 2, there is one from 2 to 1
- Complexes 1 and 2 are strongly linked if there are directed arrow pathways from 1 to 2 and from 2 to 1



Definitions

- Strong linkage class is a set of complexes for which:
  - Each pair of complexes is strongly linked
  - No complex is strongly linked to a complex outside the set

- Terminal strong linkage class: has no complex that reacts to a complex in a different strong linkage class (number = L)



A_1

$A_2 + A_3$

A_4

A_5

$2A_6$

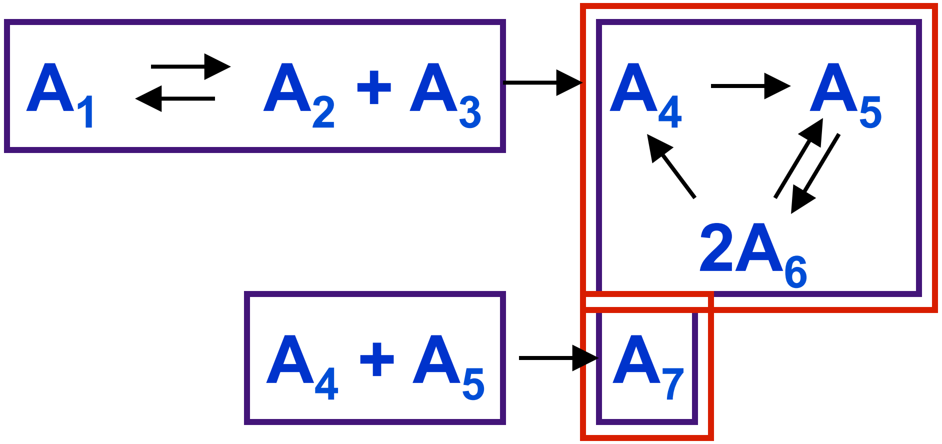
$A_4 + A_5$

A_7

Remarks

- In general, $L >= l$
- For a weakly reversible network, $L = l$

(Linkage classes, strong linkages classes, terminal strong linkage classes coincide)



Kinetics, ODE Description

- Closed, well-stirred, constant-volume, isothermal reactor

  - Can extend to open reactors by adding "pseudoreactions,"

    $0 \rightarrow A_i$, $A_i \rightarrow 0$

Species: $\{A_1, A_2, \ldots, A_N\}$

Molar concentration of A_i: $c_i \in R_{\geq 0}$

Composition vector: $c = [c_1\ c_2\ \ldots\ c_N]$

P^N = positive orthant of R^N

$\underline{P}^N$ = nonnegative orthant of R^N

Support of composition vector: $\mathbf{supp}\ c = \{A_i \mid c_i > 0\}$

Support of complex: $\mathbf{supp}\ y_i = \{A_j \mid y_{ij} > 0\}$

$\uparrow$

Stoichiometric coefficient

Kinetics, ODE Description

- Closed, well-stirred, constant-volume, isothermal reactor

Molar concentration of A_i: $c_i \in R_{\geq 0}$

Composition vector: $c = [c_1\ c_2 \ldots c_N]$

- Kinetics: An assignment to each reaction $y_i \rightarrow y_j$ of a rate function $\mathscr{K}_{i \to j}(\mathbf{c})$

  - Mass action kinetics: For each reaction $y_i \rightarrow y_j$,

$$\mathscr{K}_{i \to j}(\mathbf{c}) \equiv k_{i \to j} \prod_{L=1}^{N} (c_L)^{y_{iL}}.$$

- ODE Formulation:

$$\boxed{\dot{\mathbf{c}} = \sum_{\mathscr{R}} \mathscr{K}_{i \to j}(\mathbf{c})\,(\mathbf{y}_j - \mathbf{y}_i), \quad \mathbf{c} \in \bar{\mathbb{P}}^N}$$

Properties of ODE's

- Stoichiometric subspace $S = \{ \gamma \in \mathbb{R}^N \}$:

$$\gamma = \sum_{\mathscr{R}} \alpha_{i \to j} (\mathbf{y}_j - \mathbf{y}_i). \qquad \{\alpha_{i \to j}\}_{i \to j \in \mathscr{R}} >= 0$$

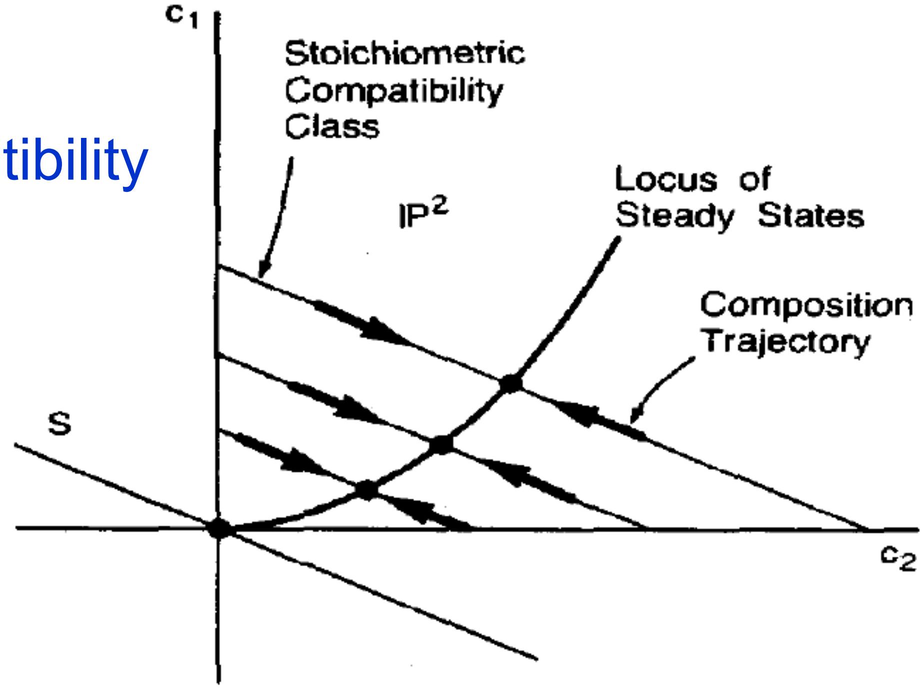
- Network rank $s = \dim(S)$

$$A_1 \rightleftarrows 2A_2$$

- $\mathbf{c}(t) - \mathbf{c}(0)$ lies in S

- Positive stoichiometric compatibility class (reaction simplex):

$$(\mathbf{c} + S) \cap \mathbb{P}^N.$$



- Goal is to classify dynamics within a stoichiometric comp. class

Steady States

- Reaction vectors are positively dependent if:

$$\mathbf{0} = \sum_{\mathscr{R}} \alpha_{i \to j} (\mathbf{y}_j - \mathbf{y}_i). \qquad \{\alpha_{i \to j}\}_{i \to j \in \mathscr{R}} > 0$$

  - Always the case in a weakly reversible network

This is a necessary condition for the existence of:

- A positive steady state $\mathbf{c}^* \in \mathbb{P}^N$ $\mathbf{0} = \sum_{\mathscr{R}} \mathscr{K}_{i \to j}(\mathbf{c}^*)(\mathbf{y}_j - \mathbf{y}_i).$
- A cyclic trajectory $\mathbf{c}(\tau) \in \mathbb{P}^N$ $\mathbf{c}(0) = \mathbf{c}(T).$

- At steady state, all reactions among complexes in a strong linkage class are switched on or off

Deficiency Zero Theorem

When $\delta = 0$:

- Network is **not** weakly reversible

  Arbitrary kinetics

  → **No** positive steady state or cyclic trajectory $\mathbf{c}(\tau) \in \mathbb{P}^N$

- Network **is** weakly reversible

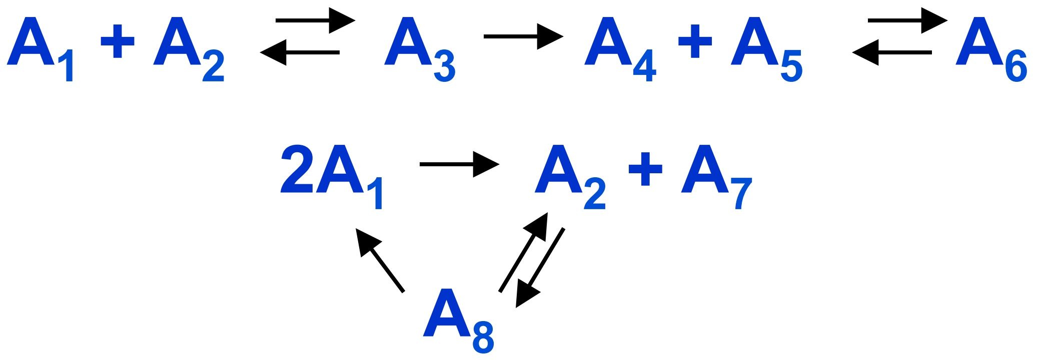
  Mass action kinetics

  → Each positive stoichiometric compatibility class has **one steady state**, which is **asymptotically stable**;

  There is no nontrivial cyclic trajectory $\mathbf{c}(\tau) \in \mathbb{P}^N$

- *Remark:* The only reactions occurring at steady state are those joining complexes in a terminal strong linkage class

Deficiency Zero Theorem: Example



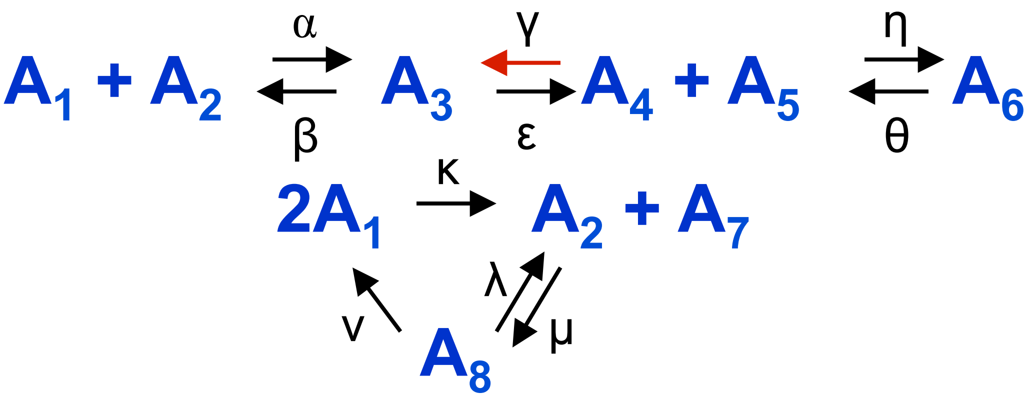
$$A_1 + A_2 \rightleftarrows A_3 \rightarrow A_4 + A_5 \rightleftarrows A_6$$

$$\begin{tikzcd}
2A_1 \arrow[rr] & & A_2 + A_7 \arrow[dl, shift left] \\
& A_8 \arrow[ul] \arrow[ur, shift left] &
\end{tikzcd}$$

$\delta = 0$, not weakly reversible

→ **No** positive steady state or cyclic trajectory $\mathbf{c}(\tau) \in \mathbb{P}^N$

Deficiency Zero Theorem: Example



$$\begin{aligned}
\dot{c}_1 &= -\alpha c_1 c_2 + \beta c_3 - 2\kappa c_1^2 + \nu c_8 \\
\dot{c}_2 &= -\alpha c_1 c_2 + \beta c_3 + \kappa c_1^2 - \lambda c_2 c_7 + \mu c_8 \\
\dot{c}_3 &= \alpha c_1 c_2 + \varepsilon c_4 c_5 - (\gamma + \beta) c_3 \\
\dot{c}_4 &= \gamma c_3 + \theta c_6 - (\varepsilon + \eta) c_4 c_5 \\
\dot{c}_5 &= \gamma c_3 + \theta c_6 - (\varepsilon + \eta) c_4 c_5 \\
\dot{c}_6 &= \eta c_4 c_5 - \theta c_6 \\
\dot{c}_7 &= \kappa c_1^2 + \mu c_8 - \lambda c_2 c_7 \\
\dot{c}_8 &= \lambda c_2 c_7 - (\mu + \nu) c_8 .
\end{aligned}$$

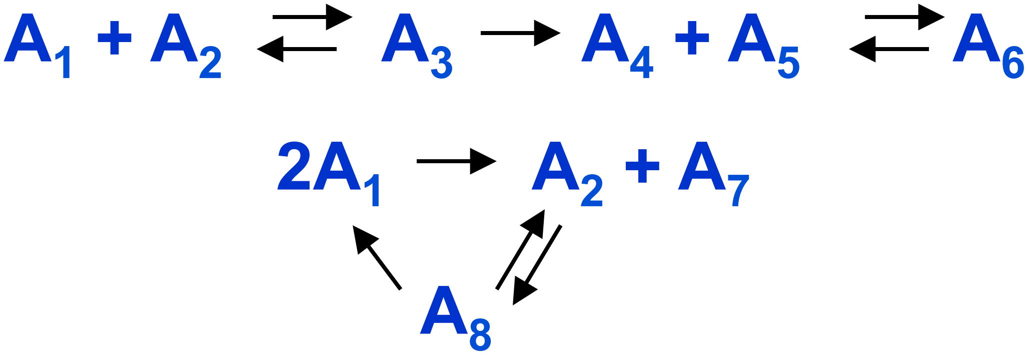
➢ Two networks with the same complexes and linkage classes have the same deficiency

→ $\delta = 0$

- Weakly reversible, assume mass action kinetics

→ System has one positive steady state, which is asymptotically stable

Remarks



$$A_1 + A_2 \rightleftarrows A_3 \rightarrow A_4 + A_5 \rightleftarrows A_6$$

$$2A_1 \rightarrow A_2 + A_7 \qquad A_2 + A_7 \rightleftarrows A_8 \qquad A_8 \rightarrow 2A_1$$

Deficiency $\delta = n - l - s$

- Two networks with the same complexes and linkage classes have the same rank → same deficiency
- Network rank <= sum of linkage class ranks
- Network deficiency >= sum of linkage class deficiencies

Deficiency One Theorem

Mass action kinetics

l linkage classes, each containing one terminal strong linkage class

(i) $\delta_\theta \leqslant 1, \quad \theta = 1, 2, \ldots, \ell$ Linkage class deficiencies

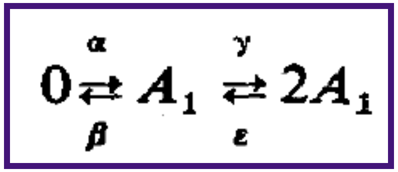
(ii) $\sum_{\theta=1}^{\ell} \delta_\theta = \delta.$ Network deficiency

→ **No more than one** steady state in a positive stoichiometric compatibility class (may depend on rate constants)

- Network is weakly reversible:

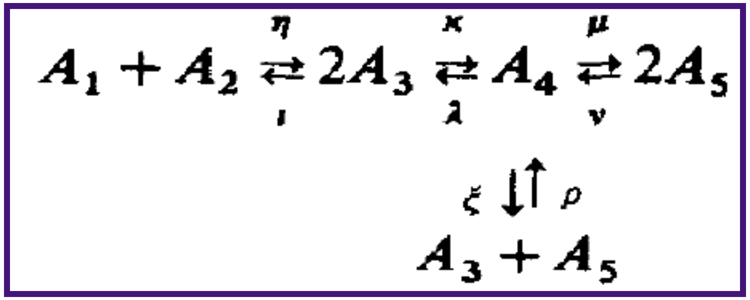
→ **Precisely one** steady state in each pos. stoich. comp. class

Deficiency One Theorem: Example

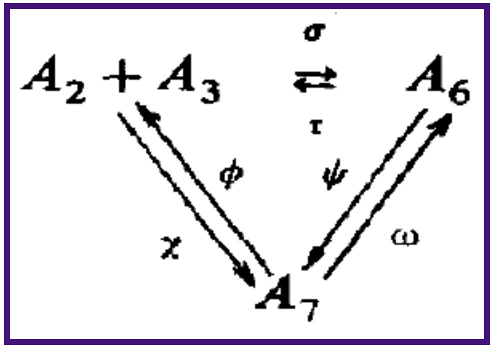


$$0 \underset{\beta}{\overset{\alpha}{\rightleftarrows}} A_1 \underset{\varepsilon}{\overset{\gamma}{\rightleftarrows}} 2A_1$$

$$\delta_1 = 1$$



$$\delta_2 = 1$$



$$\delta_3 = 0$$

$$\delta = 2 = \sum \delta_i$$

- ➢ Network is weakly reversible

→ Precisely **one** steady state in each pos. stoich. comp. class

Deficiency One Theorem: Corollary

Mass action kinetics

One linkage class

$\delta > 1$ or # of terminal strong linkage classes $L > 1$

→ Can have **multiple steady states** in a pos. stoich. comp. class

Deficiency One Theorem: Subnetworks

➢ If a set of reactions is partitioned into *p* subnetworks, then each is independent iff:

$$s = s_1 + s_2 + \ldots + s_p .$$

➢ A steady state $\mathbf{c}^*$ for a reaction network is a steady state for any independent subnetwork.

→ Can "carry down" or "carry up" information from Def. Theorems

Ex.) Network admits a positive steady state → this is a positive steady state of an independent subnetwork

Example: Single Phosphorylation

- "Futile cycle"

  ex) Signaling transduction cascades, bacterial two-component systems

Linkage classes 1 2

$$S1 + E \leftrightarrow ES1 \rightarrow S2 + E$$

$$S2 + F \leftrightarrow FS2 \rightarrow S1 + F$$

Terminal strong linkage classes

Strong linkage classes

S1 = substrate S2 = product E, F = enzymes ES1 = E bound to S1

- **Not** weakly reversible

$\delta = n - l - s = 6 - 2 - 3 = 1$ → Can't apply Deficiency Zero Theorem

$$\delta_1 = n_1 - 1 - s_1 = 3 - 1 - 2 = 0$$

$$\delta_2 = n_2 - 1 - s_2 = 3 - 1 - 2 = 0$$

$\delta_1 + \delta_2 \neq \delta$ → Can't apply Deficiency One Theorem

Deficiency One Theorem: Remarks

- Deficiency one networks that are not weakly reversible:

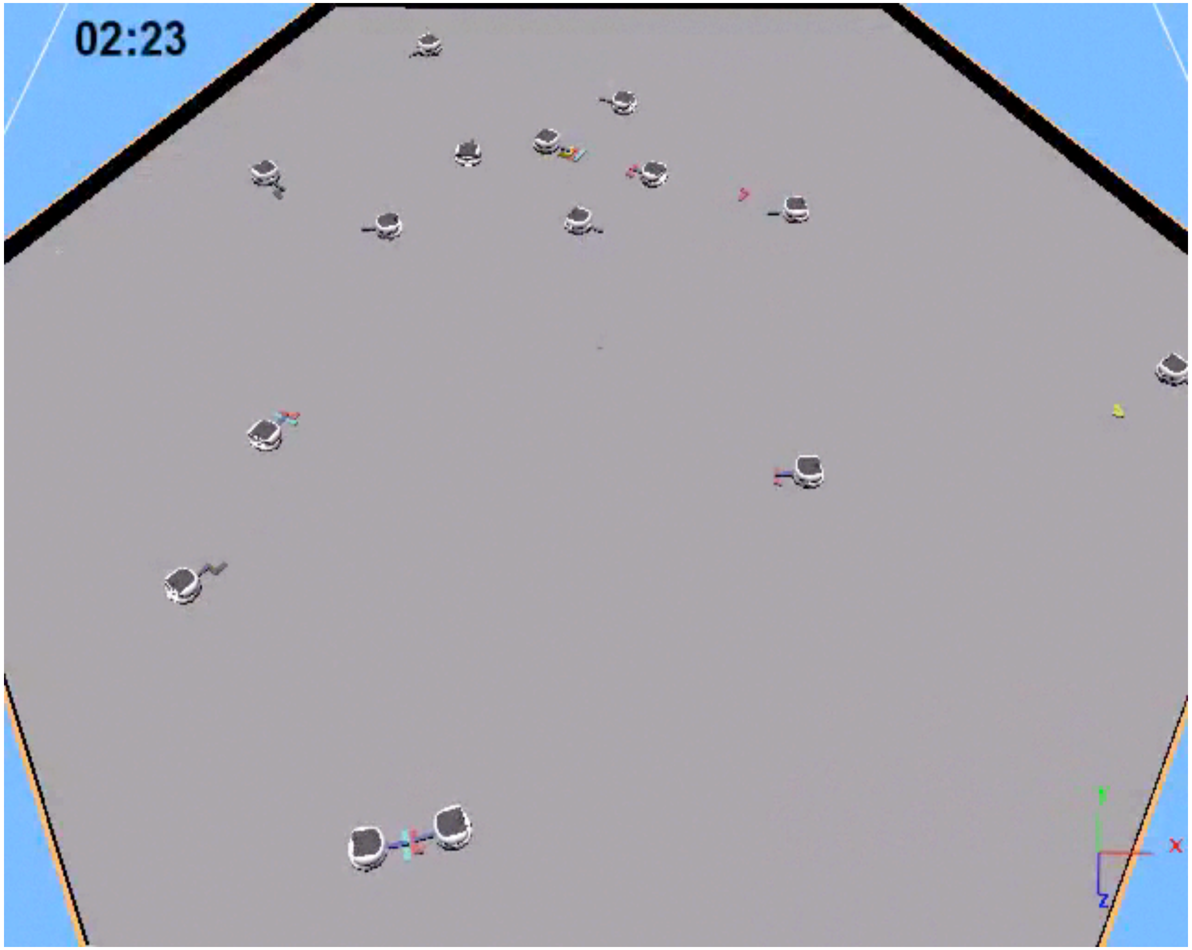
  - Can admit positive steady states for some values of rate constants *but not for others*

  - Can admit steady states in some pos. stoich. comp. classes *but not in others*

Swarm Robotic Assembly System

[Matthey, Berman, Kumar, ICRA 2009]

Design a reconfigurable manufacturing system that quickly assembles target amounts of products from a supply of heterogeneous parts



Required Robot Controller Properties

(1) Strategy should be scalable in the number of parts

Decentralized decision-making:

- Parts scattered randomly inside an arena
- Randomly moving autonomous robots assemble products
- Local sensing, local communication

(2) Minimal adjustments when product demand changes

- Probabilities of assembly and disassembly are robot control policies
- Can be updated via a broadcast

(3) System can be optimized for fast production

Spatial homogeneity → Chemical Reaction Network model

Approach

- *Ordinary differential equations*

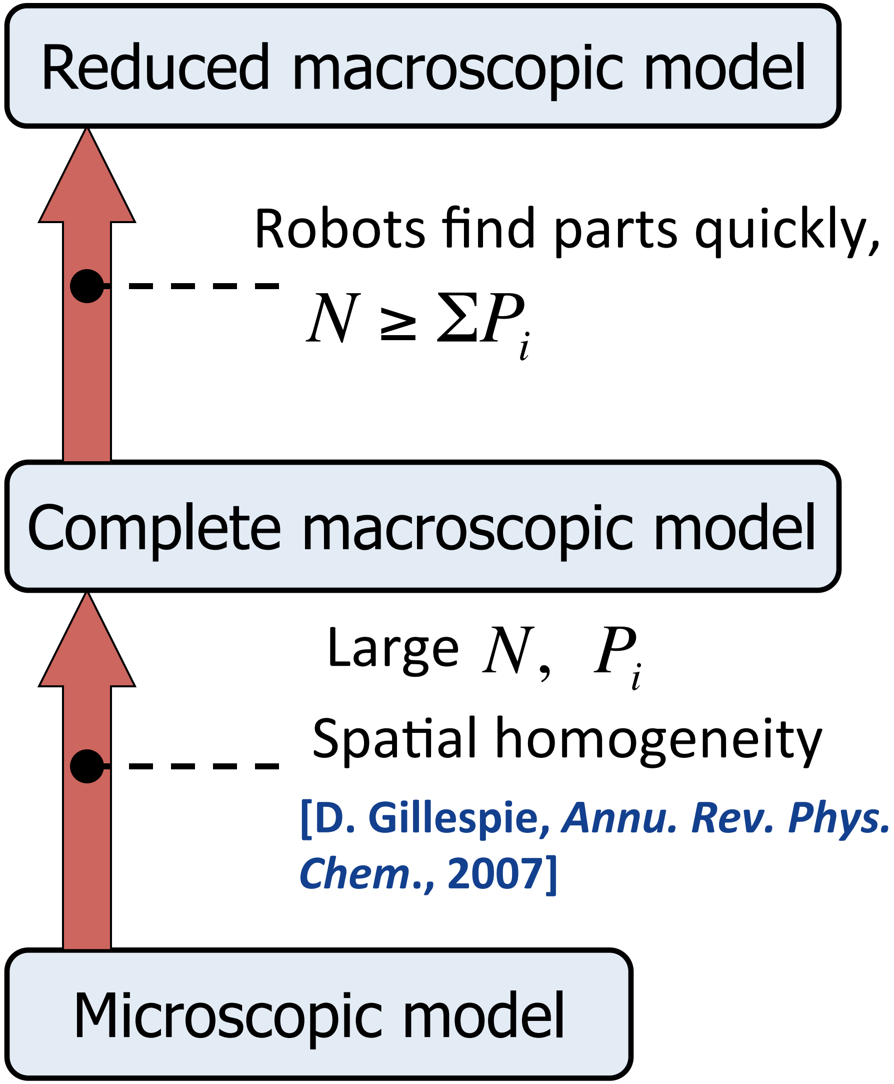
M states: continuous populations of parts

- *Ordinary differential equations*

States: continuous populations of robots and free/carried parts

- *3D physics simulation*

N robots, P_i parts;
$i = 1,\ldots,M$ types



Reduced macroscopic model

Robots find parts quickly,
$N \geq \Sigma P_i$

Complete macroscopic model

Large N, P_i

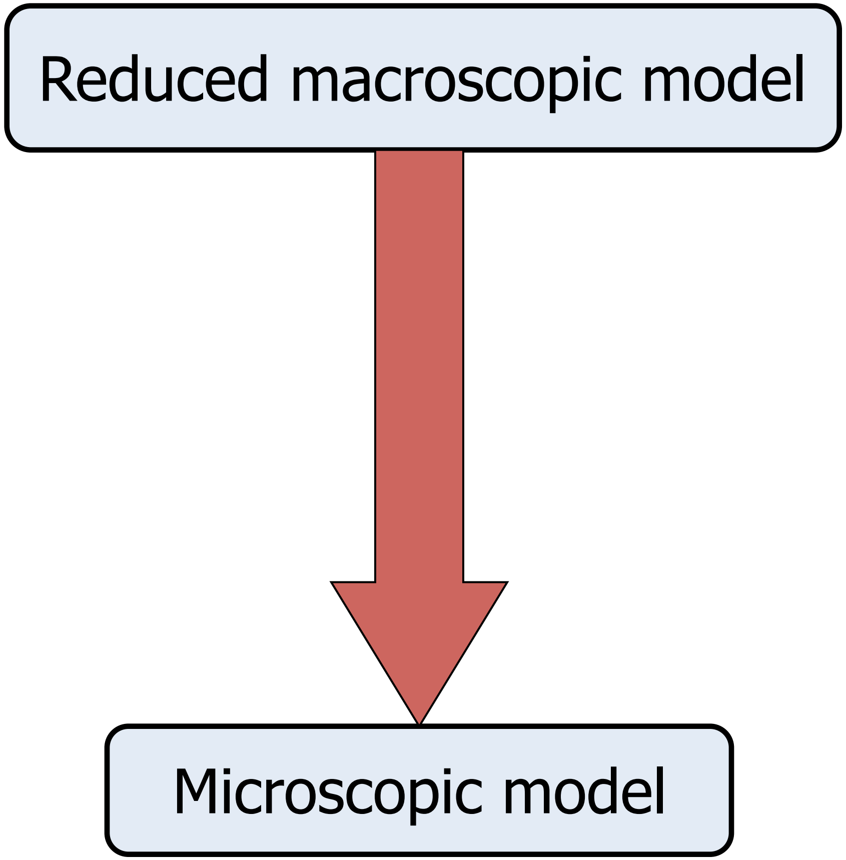
Spatial homogeneity

[D. Gillespie, *Annu. Rev. Phys. Chem.*, 2007]

Microscopic model

Approach

ODEs are functions of probabilities of assembly and disassembly:
Optimize for fast assembly of target amounts of products



Reduced macroscopic model

Microscopic model

Robots start assemblies and perform disassemblies according to optimized probabilities

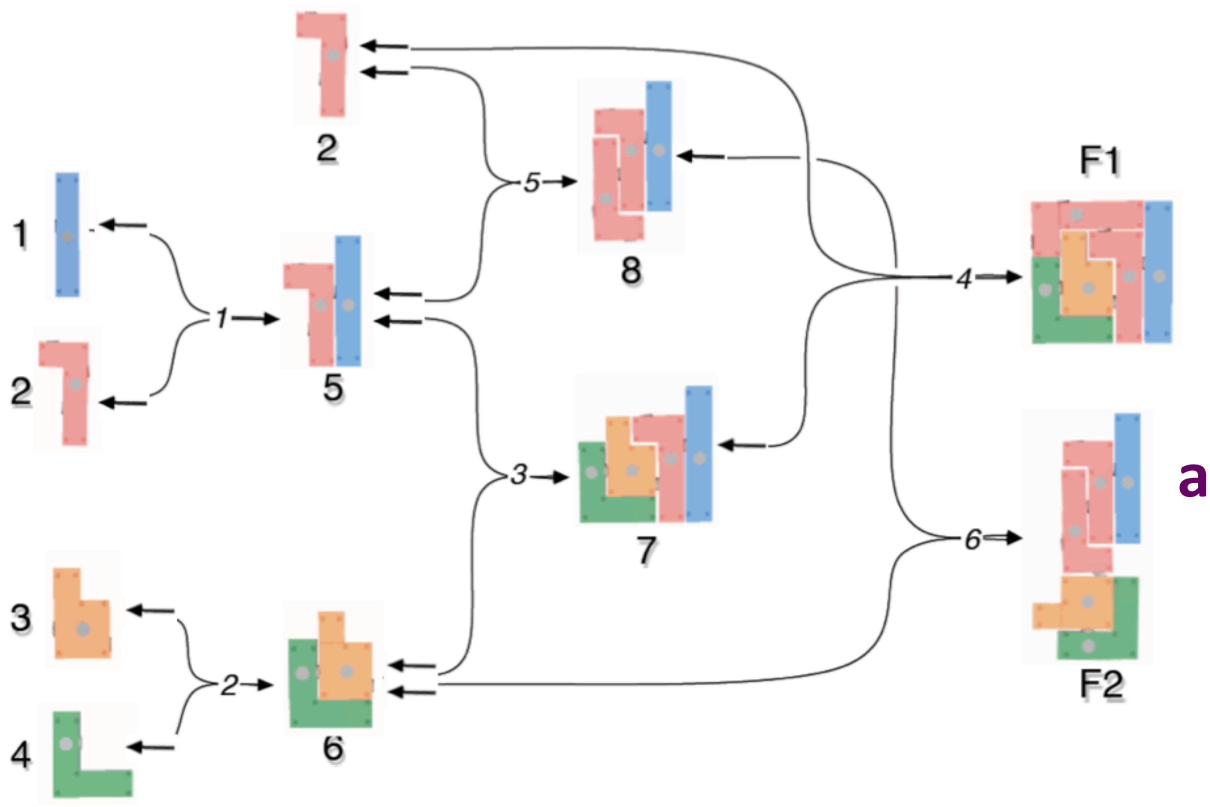
Example

- Implemented in the robot simulator Webots (www.cyberbotics.com)

  - Uses Open Dynamics Engine to simulate physics

- Predefined assembly plan:

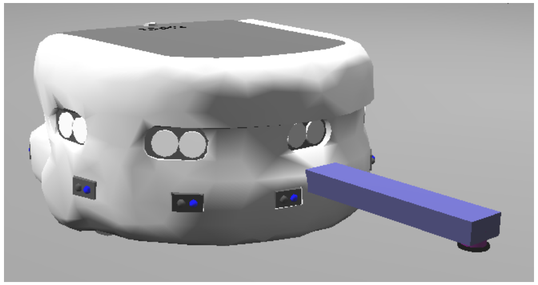
4 types of **basic parts**

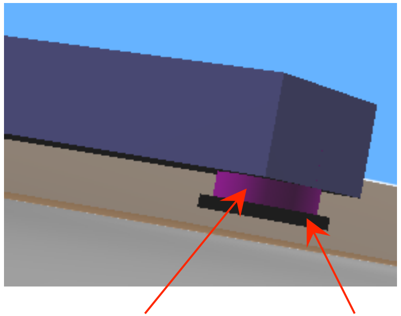


2 types of **final assemblies**

Example

Khepera III + bar
(www.k-team.com)

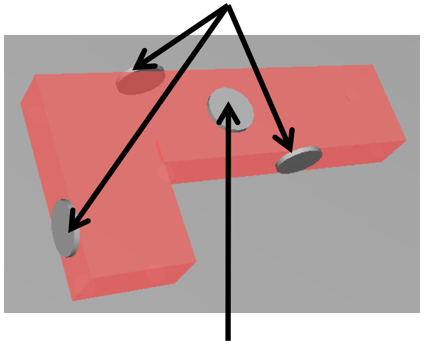




Rotational servo

Magnet

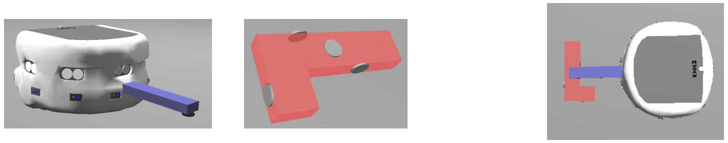
Magnets that bond to other parts



Bonds to bar

- Magnets can be turned on or off
- Servo rotates bonded part to orientation for assembly
- Infra-red distance sensors for collision avoidance
- Emitter/receiver on each robot and basic part for local communication, computing relative bearing

Decisions Modeled as Chemical Reactions

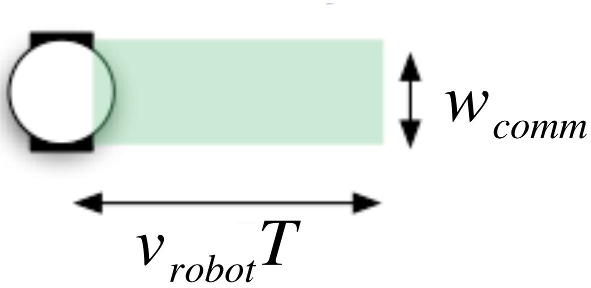


$$X_R + X_i^u \xrightarrow{e_i} X_i^c \qquad i = 1, ..., 8$$

$$X_l^c + X_m^c \xrightarrow{k_j^+} X_n^c + X_R \qquad\qquad X_n^c \xrightarrow{k_j^-} X_l^c + X_m^u$$

$$\boxed{e_i = A \enclose{circle}{p^e}, \qquad k_j^+ = A \enclose{circle}{p^e}\, p_j^a \; p_j^+ \;, \qquad k_j^- = p_j^-}$$

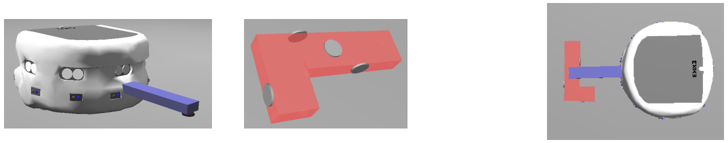
p^e = prob. that a robot encounters a part or another robot $\approx \dfrac{v_{robot} T w_{comm}}{A}$



[Correll and Martinoli, Coll. Beh. Workshop, ICRA 2007]

A = arena area

Decisions Modeled as Chemical Reactions



$$X_R + X_i^u \xrightarrow{e_i} X_i^c \qquad i = 1, ..., 8$$

$$X_l^c + X_m^c \xrightarrow{k_j^+} X_n^c + X_R$$

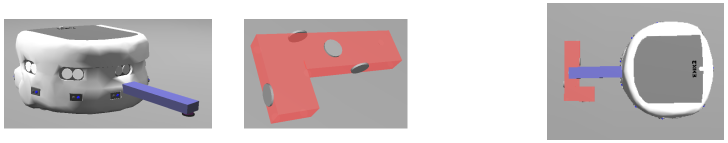
$$X_n^c \xrightarrow{k_j^-} X_l^c + X_m^u$$

$$\boxed{e_i = A\, p^e \ , \qquad k_j^+ = A\, p^e\, p_j^a\, p_j^+ \ , \qquad k_j^- = p_j^-}$$

p_j^a = prob. of two robots successfully completing assembly process *j*

(measured from simulations)

Decisions Modeled as Chemical Reactions



$$X_R + X_i^u \xrightarrow{e_i} X_i^c \qquad i = 1, ..., 8$$

$$X_l^c + X_m^c \xrightarrow{k_j^+} X_n^c + X_R$$

$$X_n^c \xrightarrow{k_j^-} X_l^c + X_m^u$$

$$\boxed{e_i = A\ p^e\ , \qquad k_j^+ = A\ p^e\ p_j^a\, p_j^+\ , \qquad k_j^- = p_j^-}$$

Tunable:

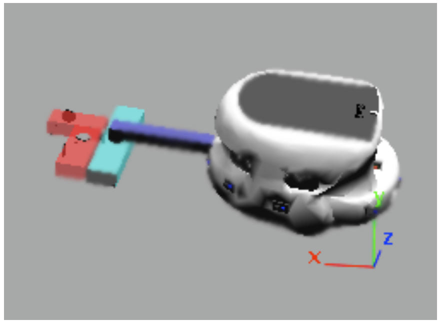
p_j^+ = prob. of two robots starting assembly process *j*

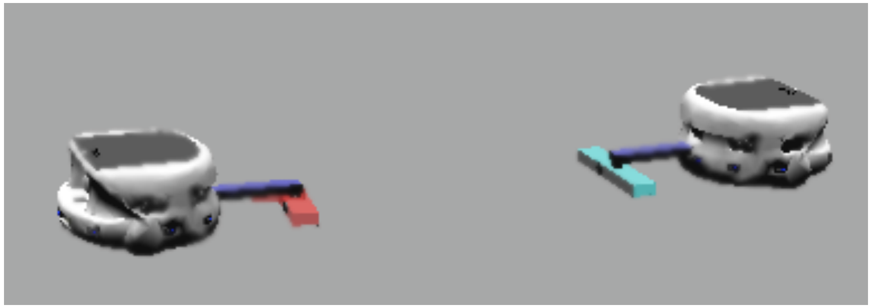
p_j^- = prob. per unit time of a robot performing disassembly process *j*

Mapping p_i^+, p_i^- onto the Robot Controllers

Δt = simulation timestep (32 ms)

u = random number uniformly distributed over [0,1]





Robot computes u at each Δt, disassembles the part if

$$u < p_i^- \Delta t$$

Robot computes u, executes assembly if

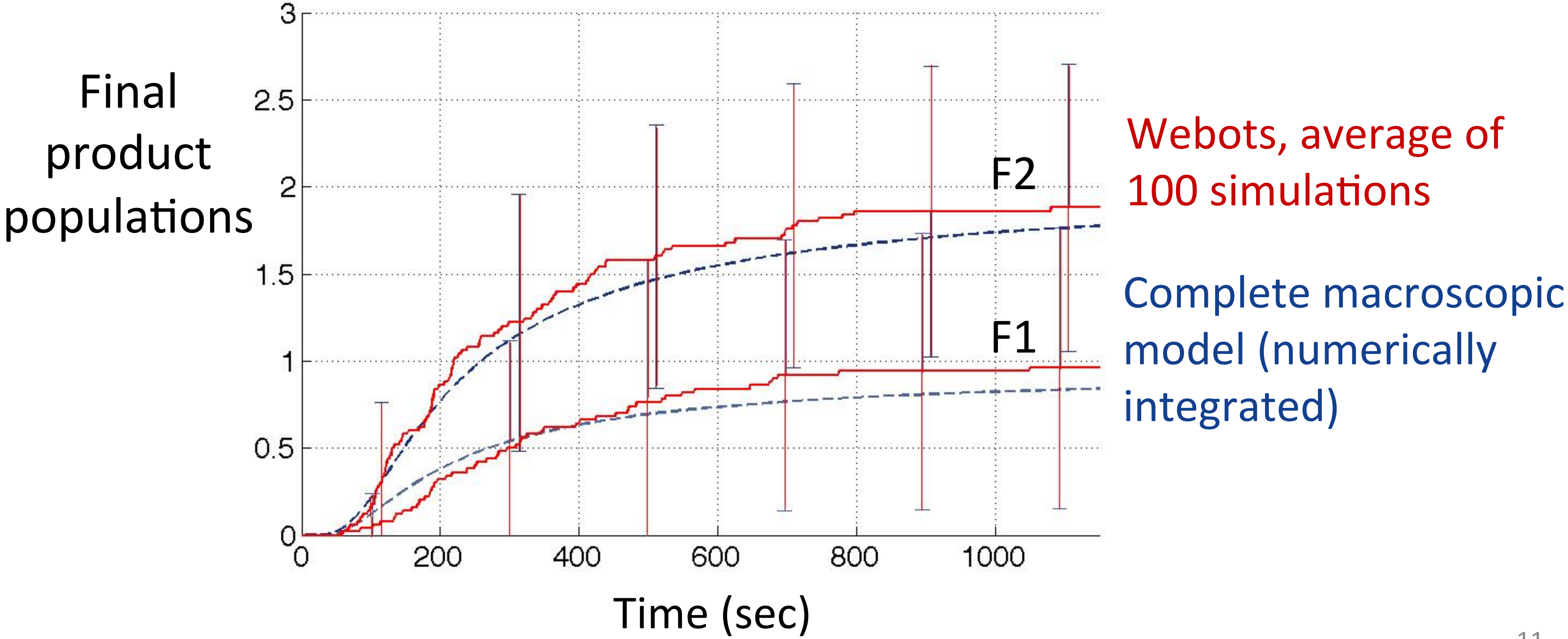
$$u < p_i^+$$

Validation of Complete Macroscopic Model

- Macroscopic model (set of ODEs) is fairly accurate
- Discrepancies are due to:

Relatively low populations; ODE most accurate for large ones

Assembly disruption in simulation (not modeled)



Reduced Macroscopic Model

Lower-dimensional model (abstract away robots):

$$\boxed{X_1 + X_2} \underset{k_1^-}{\overset{k_1^+}{\rightleftharpoons}} \boxed{X_5} \qquad X_3 + X_4 \underset{k_2^-}{\overset{k_2^+}{\rightleftharpoons}} X_6 \qquad X_5 + X_6 \underset{k_3^-}{\overset{k_3^+}{\rightleftharpoons}} X_7$$

$$X_2 + X_7 \underset{k_4^-}{\overset{k_4^+}{\rightleftharpoons}} X_{F1} \qquad X_2 + X_5 \underset{k_5^-}{\overset{k_5^+}{\rightleftharpoons}} X_8 \qquad X_6 + X_8 \underset{k_6^-}{\overset{k_6^+}{\rightleftharpoons}} X_{F2}$$

Vector of complexes:

$$\mathbf{y}(\mathbf{x}) = [x_1x_2 \quad x_5 \quad x_3x_4 \quad x_6 \quad x_2x_7 \quad x_{F1} \quad x_5x_6 \quad x_7 \quad x_2x_5 \quad x_8 \quad x_6x_8 \quad x_{F2}]^T$$

$$\boxed{\dot{\mathbf{x}} = \mathbf{MKy}(\mathbf{x})}$$

We also define a matrix $\mathbf{M} \in \mathbb{R}^{10\times 12}$ in which each entry $\mathbf{M}_{ji}$, $j = 1, ..., 10$, of column $\mathbf{m}_i$ is the coefficient of part type j in complex i (0 if absent). We relabel the rate associated with reaction $(i, j) \in \mathcal{E}$ as k_{ij} and define a matrix $\mathbf{K} \in \mathbb{R}^{12\times 12}$ with entries

$$\mathbf{K}_{ij} = \begin{cases} k_{ji} & \text{if} \quad i \neq j\ , \quad (j,i) \in \mathcal{E}\ , \\ 0 & \text{if} \quad i \neq j\ , \quad (j,i) \notin \mathcal{E}\ , \\ -\sum_{(i,l)\in\mathcal{E}} k_{il} & \text{if} \quad i = j\ . \end{cases} \qquad (5)$$

Conservation constraints:

$$\begin{aligned} x_3 - x_4 &= N_1 \\ x_1 + x_5 + x_7 + x_8 + x_{F1} + x_{F2} &= N_2 \\ x_2 + x_5 + x_7 + 2(x_8 + x_{F1} + x_{F2}) &= N_3 \\ x_3 + x_6 + x_7 + x_{F1} + x_{F2} &= N_4 \end{aligned}$$

Reduced Macroscopic Model

$$\boxed{\dot{\mathbf{x}} = \mathbf{MKy}(\mathbf{x})}$$

$$\begin{aligned} x_3 - x_4 &= N_1 \\ x_1 + x_5 + x_7 + x_8 + x_{F1} + x_{F2} &= N_2 \\ x_2 + x_5 + x_7 + 2(x_8 + x_{F1} + x_{F2}) &= N_3 \\ x_3 + x_6 + x_7 + x_{F1} + x_{F2} &= N_4 \end{aligned}$$

The system has a unique, positive, globally asymptotically stable equilibrium.

Proof: Reaction network is *deficiency zero* and *weakly reversible*, does not admit equilibria with some $x_i = 0$

→ We can design $\mathbf{K}$ such that the system always converges to a target equilibrium, $\mathbf{x^d} > \mathbf{0}$