Flux coupling relations (reminder)

Burgard et al. 04

- $C = \{v \mid Sv = 0,\ v_k \geq 0, k \in Irr\}$ flux cone
- A reaction i is blocked if $v_i = 0$, for all $v \in C$.
- Let i and j be two unblocked reactions.
  - i is directionally coupled to j, $i \overset{=0}{\rightarrow} j$, if for all $v \in C$, $v_i = 0$ implies $v_j = 0$.
  - i and j are partially coupled, $i \overset{=0}{\leftrightarrow} j$, if for all $v \in C$, $v_i = 0$ is equivalent to $v_j = 0$.
  - i and j are fully coupled, $i \backsim^{\lambda} j$, if there exists $\lambda \in \mathbb{R} \setminus \{0\}$ such that for all $v \in C, v_j = \lambda v_i$.

Flux coupling and EFMs

Marashi/Bockmayr 11

Proposition
Let $\mathscr{N}$ be a metabolic network with flux cone C and set of elementary modes E.

For any two reactions i and j, the following are equivalent:

(i) For all $v \in C$, $v_i = 0$ implies $v_j = 0$.
(ii) For all $e \in E$, $e_i = 0$ implies $e_j = 0$.

Flux coupling and EFMs (ctd)

Corollary
Let i, j be two non-blocked reactions in a metabolic network $\mathscr{N}$ with set of elementary modes E. Then:

- $i \overset{=0}{\rightarrow} j$ iff for all $e \in E$, $e_i = 0$ implies $e_j = 0$.
- $i \overset{=0}{\leftrightarrow} j$ iff for all $e \in E$, $e_i = 0$ is equivalent to $e_j = 0$.
- $i \backsim^{\lambda} j$ iff there exists $\lambda \neq 0$ such that for all $e \in E$, $e_j = \lambda \cdot e_i$.

Flux uncoupling

- Two reactions i, j are uncoupled if neither $i \overset{=0}{\rightarrow} j$ nor $j \overset{=0}{\rightarrow} i$.
- Equivalently, there exist EFMs $e, e' \in E$ such that

$$e_i = 0,\ e_j \neq 0 \quad \text{and} \quad e'_i \neq 0,\ e'_j = 0.$$

- Two uncoupled reactions i, j are called mutually exclusive if there is no EFM $e \in E$ with

$$e_i \neq 0,\ \ e_j \neq 0.$$

(i and j never occur together in the same EFM).