Discretization and Equivalences in Bio-PEPA

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Discretisation and Equivalence in Bio-PEPA

Outline

Bio-PEPA

Syntax and semantics

Equivalence choice

Equivalence definition

Results

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Bio-PEPA	Syntax and semantics	Equivalence definition	
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- Bio-PEPA systems with finite number of levels, CTMCs

sequential component, species

$${old S}::=\ (lpha,\kappa) ext{ op } {old S} \ | \ {old S}+{old S} ext{ op } \in \{ \uparrow, \downarrow, \oplus, \ominus, \odot \}$$

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$$P ::= S(\ell) \mid P \bowtie_L P$$

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$$P ::= \frac{S(\ell)}{P \bowtie_{L} P}$$

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$$\mathcal{S} ::= (\alpha, \kappa) \text{ op } \mathcal{S} \mid \mathcal{S} + \mathcal{S} \qquad \text{ op } \in \{\uparrow, \downarrow, \oplus, \ominus, \odot \}$$

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$$\blacktriangleright P \stackrel{\text{\tiny def}}{=} C_1(\ell_1) \underset{\ell_1}{\bowtie} \dots \underset{\ell_{m-1}}{\bowtie} C_m(\ell_m) \text{ with all } C_i\text{'s distinct}$$

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Example: reaction with enzyme $\blacktriangleright S + E \stackrel{\longrightarrow}{\leftarrow} SE \stackrel{\longrightarrow}{\rightarrow} P + E$

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$$\blacktriangleright S + E \stackrel{\longrightarrow}{\longleftarrow} SE \longrightarrow P + E$$

• $S(\ell_S) \bowtie E(\ell_E) \bowtie SE(\ell_{SE}) \bowtie P(\ell_P)$ where

$$\triangleright S + E \underset{\longleftarrow}{\longrightarrow} SE \longrightarrow P + E$$

• $S(\ell_S) \boxtimes E(\ell_E) \boxtimes SE(\ell_{SE}) \boxtimes P(\ell_P)$ where

$$\begin{split} S &\stackrel{\text{def}}{=} (\alpha, 1) \downarrow S + (\beta, 1) \uparrow S \\ E &\stackrel{\text{def}}{=} (\alpha, 1) \downarrow E + (\beta, 1) \uparrow E + (\gamma, 1) \uparrow E \\ SE &\stackrel{\text{def}}{=} (\alpha, 1) \uparrow SE + (\beta, 1) \downarrow SE + (\gamma, 1) \downarrow SE \\ P &\stackrel{\text{def}}{=} (\gamma, 1) \uparrow P \end{split}$$

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 $\triangleright S \xrightarrow{E} P$

Michaelis-Menten kinetics

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► $S \xrightarrow{E} P$ Michaelis-Menten kinetics ► $S(\ell_S) \Join E(\ell_E) \Join P(\ell_P)$ where $S \stackrel{def}{=} (\delta, 1) \downarrow S \quad E \stackrel{def}{=} (\delta, 1) \oplus E \quad P \stackrel{def}{=} (\delta, 1) \uparrow P$

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Bio-PEPA system

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 - P is a well-defined model component

Bio-PEPA systems with levels

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- obtain CTMCs from operational semantics

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 \blacktriangleright operational semantics for capability relation \rightarrow_c

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- \blacktriangleright operational semantics for capability relation \rightarrow_c
- Prefix rules

 $((\alpha,\kappa) \downarrow S)(\ell) \xrightarrow{(\alpha,[S: \downarrow (\ell,\kappa)])} S(\ell-\kappa) \quad \kappa \leq \ell \leq N_S$ $((\alpha,\kappa)\uparrow S)(\ell) \xrightarrow{(\alpha,[S:\uparrow(\ell,\kappa)])} S(\ell+\kappa) \quad 0 \leq \ell \leq N_S - \kappa$ $((\alpha,\kappa)\oplus S)(\ell) \xrightarrow{(\alpha,[S:\oplus(\ell,\kappa)])} S(\ell)$ $0 < \ell < N_S$ $((\alpha,\kappa)\ominus S)(\ell) \xrightarrow{(\alpha,[S:\ominus(\ell,\kappa)])} S(\ell)$ $0 < \ell < N_S$ $((\alpha, \kappa) \odot S)(\ell) \xrightarrow{(\alpha, [S: \odot(\ell, \kappa)])} S(\ell)$ $0 < \ell < N_S$

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 $((\alpha,\kappa) \downarrow S)(\ell) \xrightarrow{(\alpha,[S: \downarrow (\ell,\kappa)])} S(\ell-\kappa) \quad \kappa \leq \ell \leq N_S$ $((\alpha,\kappa)\uparrow S)(\ell) \xrightarrow{(\alpha,[S:\uparrow(\ell,\kappa)])} S(\ell+\kappa) \quad 0 \leq \ell \leq N_S - \kappa$ $((\alpha,\kappa)\oplus S)(\ell) \xrightarrow{(\alpha,[S:\oplus(\ell,\kappa)])} S(\ell)$ $0 < \ell < N_S$ $((\alpha,\kappa) \ominus S)(\ell) \xrightarrow{(\alpha,[S:\ominus(\ell,\kappa)])} S(\ell)$ $0 < \ell < N_S$ $((\alpha, \kappa) \odot S)(\ell) \xrightarrow{(\alpha, [S: \odot(\ell, \kappa)])} S(\ell)$ $0 < \ell < N_S$

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Constant

$$\frac{S(\ell) \xrightarrow{(\alpha,w)} c S'(\ell')}{C(\ell) \xrightarrow{(\alpha,w)} c S'(\ell')} \quad C \stackrel{def}{=} S$$

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Constant

$$\frac{S(\ell) \xrightarrow{(\alpha,w)} c S'(\ell')}{C(\ell) \xrightarrow{(\alpha,w)} c S'(\ell')} \quad C \stackrel{\text{\tiny def}}{=} S$$

$$\frac{S_1(\ell) \xrightarrow{(\alpha,w)}_c S'(\ell')}{(S_1 + S_2)(\ell) \xrightarrow{(\alpha,w)}_c S'(\ell')} \quad \frac{S_2(\ell) \xrightarrow{(\alpha,w)}_c S'(\ell')}{(S_1 + S_2)(\ell) \xrightarrow{(\alpha,w)}_c S'(\ell')}$$

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► Constant $\frac{S(\ell) \xrightarrow{(\alpha,w)} c S'(\ell')}{C(\ell) \xrightarrow{(\alpha,w)} c S'(\ell')} \quad C \stackrel{\text{def}}{=} S$

Choice

$$\frac{S_1(\ell) \xrightarrow{(\alpha,w)}_c S'(\ell')}{(S_1 + S_2)(\ell) \xrightarrow{(\alpha,w)}_c S'(\ell')} \quad \frac{S_2(\ell) \xrightarrow{(\alpha,w)}_c S'(\ell')}{(S_1 + S_2)(\ell) \xrightarrow{(\alpha,w)}_c S'(\ell')}$$

• Cooperation for $\alpha \not\in L$

$$\frac{P \xrightarrow{(\alpha,w)}_{c} P'}{P \bowtie_{L} Q \xrightarrow{(\alpha,w)}_{c} P' \bowtie_{L} Q} \qquad \frac{Q \xrightarrow{(\alpha,w)}_{c} Q'}{P \bowtie_{L} Q \xrightarrow{(\alpha,w)}_{c} P \bowtie_{L} Q'}$$

• Cooperation for $\alpha \in L$

$$\frac{P \xrightarrow{(\alpha, \mathbf{V})}_{c} P' \quad Q \xrightarrow{(\alpha, \mathbf{U})}_{c} Q'}{P \bigotimes_{L} Q \xrightarrow{(\alpha, \mathbf{V} :: \mathbf{U})}_{c} P' \bigotimes_{L} Q'} \quad \alpha \in L$$

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• operational semantics for stochastic relation \rightarrow_s

$$\frac{P \xrightarrow{(\alpha, v)} c P'}{(\alpha, \mathcal{K}, \mathcal{F}, \mathsf{Comp}, P)} \xrightarrow{(\alpha, f_{\alpha}(v, \mathcal{N}, \mathcal{K})/h)} s \langle \mathcal{V}, \mathcal{N}, \mathcal{K}, \mathcal{F}, \mathsf{Comp}, P' \rangle$$

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Discretisation and Equivalence in Bio-PEPA

▶ Cooperation for $\alpha \in L$

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• qualitative, only consider α

Example: reaction with enzyme, max level 3

▶ state vector (S, E, SE, P) and $N_S = N_E = N_{SE} = N_P = 3$

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Example: reaction with enzyme, max level 3

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Example: reaction with enzyme, max level 7

▶ state vector *S E SE P* and $N_S = N_E = N_{SE} = N_P = 7$

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Example: reaction with enzyme, max level 7

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modelling with levels leads to different discretisations

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 $P^n \equiv P^m$ for certain *m* and *n*

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 $P^n \equiv P^m$ for certain *m* and *n*

prove it is a congruence for relevant operators

 $P_1 \equiv P_2$ and $Q_1 \equiv Q_2$ implies $P_1 \parallel Q_1 \equiv P_2 \parallel Q_2$

Approach taken

aim for a bisimulation-style equivalence

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Discretisation and Equivalence in Bio-PEPA

Bio-PEPA	Syntax and semantics	Equivalence choice	Equivalence definition	Results
Approad	ch taken			
► a	im for a bisimulatio	n-style equivalence	9	

- y 4

► bisimilarity,
$$P \sim Q$$
 if
1. $P \xrightarrow{(\alpha,v)}_{c} P'$, $Q \xrightarrow{(\alpha,u)}_{c} Q'$ and $P' \sim Q'$
2. $Q \xrightarrow{(\alpha,u)}_{c} Q'$, $P \xrightarrow{(\alpha,v)}_{c} P'$ and $P' \sim Q'$

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- approach taken
 - determine definition of equivalence

Bio-PEPA	Syntax and semantics	Equivalence choice	Equivalence definition	Results
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- aim for a bisimulation-style equivalence
 - \blacktriangleright bisimilarity, $P \sim Q$ if 1. $P \xrightarrow{(\alpha,\nu)} P'$. $Q \xrightarrow{(\alpha,u)} Q'$ and $P' \sim Q'$ 2. $Q \xrightarrow{(\alpha, u)} Q' P \xrightarrow{(\alpha, v)} P'$ and $P' \sim Q'$
 - approach taken
 - determine definition of equivalence
 - prove it relates to two discretisations of a single species

句

aim for a bisimulation-style equivalence

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approach taken

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approach taken

- determine definition of equivalence
- prove it relates to two discretisations of a single species
- prove it is a congruence for cooperation operator
- prove that it relates two discretisations of a system with many species

$$\blacktriangleright B \stackrel{\scriptscriptstyle def}{=} (\alpha, \ 3 \) \downarrow B \ + \ (\beta, \ 4 \) \uparrow B \ + \ (\gamma, 1) \uparrow B$$



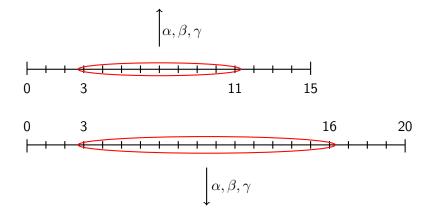
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$$\blacktriangleright B \stackrel{\text{\tiny def}}{=} (\alpha, \mathbf{3}) \downarrow B + (\beta, \mathbf{4}) \uparrow B + (\gamma, 1) \uparrow B$$



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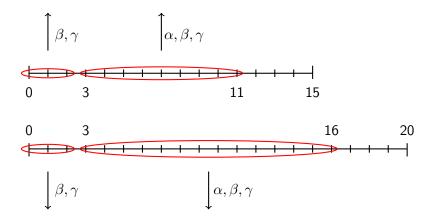
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Discretisation and Equivalence in Bio-PEPA

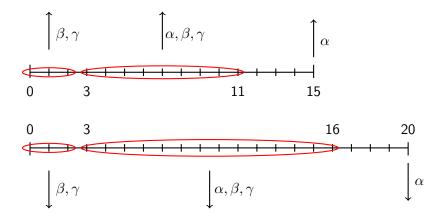
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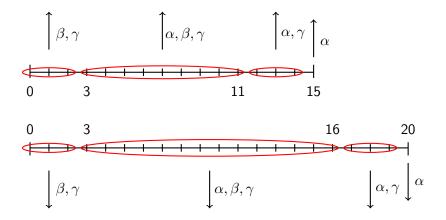
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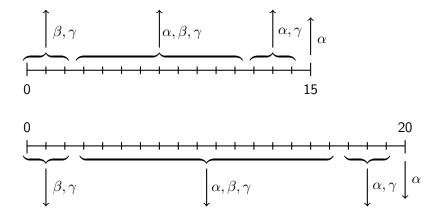
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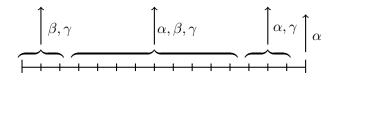
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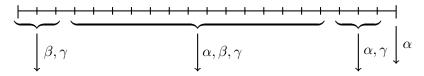


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Discretisation and Equivalence in Bio-PEPA

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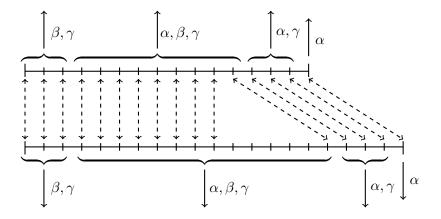




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Discretisation and Equivalence in Bio-PEPA

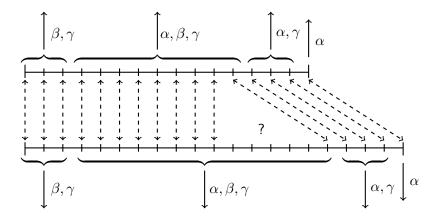
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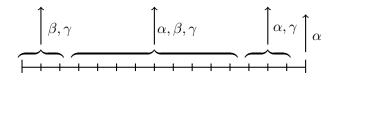
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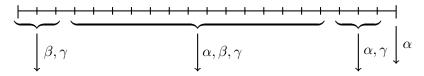


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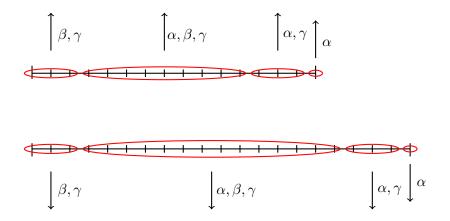




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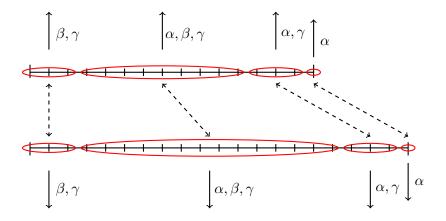
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Discretisation and Equivalence in Bio-PEPA

▶ $(P, Q) \in \mathcal{H}$ if they can perform the same actions

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Discretisation and Equivalence in Bio-PEPA

- ▶ $(P, Q) \in \mathcal{H}$ if they can perform the same actions
- \mathcal{H} is an equivalence relation

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•
$$[P] \xrightarrow{\alpha} [Q] \text{ if } P \xrightarrow{(\alpha, v)} _{c} Q$$

- ▶ $(P, Q) \in \mathcal{H}$ if they can perform the same actions
- \blacktriangleright ${\cal H}$ is an equivalence relation

$$\blacktriangleright [P] \stackrel{\alpha}{\hookrightarrow} [Q] \text{ if } P \stackrel{(\alpha, v)}{\longrightarrow}_{c} Q$$

base equivalence on standard bisimilarity

- ▶ $(P, Q) \in \mathcal{H}$ if they can perform the same actions
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$$\blacktriangleright [P] \stackrel{\alpha}{\hookrightarrow} [Q] \text{ if } P \stackrel{(\alpha, v)}{\longrightarrow}_{c} Q$$

- base equivalence on standard bisimilarity
- compression bisimilarity, P ≏ Q if [P] ~ [Q], namely if
 1. [P] → [P'], [Q] → [Q'] and [P'] ~ [Q']
 2. [Q] → [Q'], [P] → [P'] and [P'] ~ [Q']

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- base equivalence on standard bisimilarity
- ► compression bisimilarity, $P \simeq Q$ if $[P] \sim [Q]$, namely if 1. $[P] \stackrel{\alpha}{\longrightarrow} [P']$, $[Q] \stackrel{\alpha}{\longrightarrow} [Q']$ and $[P'] \sim [Q']$ 2. $[Q] \stackrel{\alpha}{\longrightarrow} [Q']$, $[P] \stackrel{\alpha}{\longrightarrow} [P']$ and $[P'] \sim [Q']$

• equivalence classes: *n* levels, E_1, \ldots, E_p ; *m* levels, F_1, \ldots, F_q

- ▶ $(P, Q) \in \mathcal{H}$ if they can perform the same actions
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- maximum stoichiometry for reactant: k_{\downarrow}

句

Equivalence definition

- ▶ $(P, Q) \in \mathcal{H}$ if they can perform the same actions
- \mathcal{H} is an equivalence relation

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- equivalence classes: *n* levels, E_1, \ldots, E_p ; *m* levels, F_1, \ldots, F_q
- maximum stoichiometry for reactant: k_{\downarrow}
- ► maximum stoichiometry for product: k_↑

Bio-PEPA	Syntax and semantics		Equivalence definition	Results				
Results								
► for a well-defined Bio-PEPA species, $C^n \simeq C^m$ if								
<i>n</i> ,	$k_{\downarrow},m\geq k_{\downarrow}+\max\{k_{\downarrow}\}$	$,k_{\uparrow}\}+k_{\uparrow}$						

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BIO-PEPA	Syntax and semantics	Equivalence choice	Equivalence definition	Results				
Results								
 for a well-defined Bio-PEPA species, Cⁿ ≃ C^m if n, m ≥ k_↓ + max{k_↓, k_↑} + k_↑ 								
 equivalence classes are intervals and hence ordered 								

Bio-PEPA	Syntax and semantics			Results			
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 - transition-preserving isomorphism between equivalence classes
 - equivalence classes are bisimilar

- CADP: current action decomposition property
 - ▶ $(P_1 \bowtie Q_1, P_2 \bowtie Q_2) \in \mathcal{H}$ and derivatives of same model then $(P_1, P_2) \in \mathcal{H}, (Q_1, Q_2) \in \mathcal{H}$

- CADP: current action decomposition property
 - ▶ $(P_1 \bowtie Q_1, P_2 \bowtie Q_2) \in \mathcal{H}$ and derivatives of same model then $(P_1, P_2) \in \mathcal{H}, (Q_1, Q_2) \in \mathcal{H}$
- ▶ if $P_1 \simeq P_2$, $Q_1 \simeq Q_2$ and $P_1 \bowtie_L Q_1$ has CADP and $P_2 \bowtie_L Q_2$ has CADP then $P_1 \bowtie_l Q_1 \simeq P_2 \bowtie_l Q_2$

- CADP: current action decomposition property
 - ▶ $(P_1 \bowtie Q_1, P_2 \bowtie Q_2) \in \mathcal{H}$ and derivatives of same model then $(P_1, P_2) \in \mathcal{H}, (Q_1, Q_2) \in \mathcal{H}$
- ▶ if $P_1 \simeq P_2$, $Q_1 \simeq Q_2$ and $P_1 \bowtie Q_1$ has CADP and $P_2 \bowtie Q_2$ has CADP then $P_1 \bowtie Q_1 \simeq P_2 \bowtie Q_2$

► $(P_1, P_2) \in \mathcal{H}$ then $(P_1 \Join_l Q, P_2 \Join_l Q) \in \mathcal{H}$

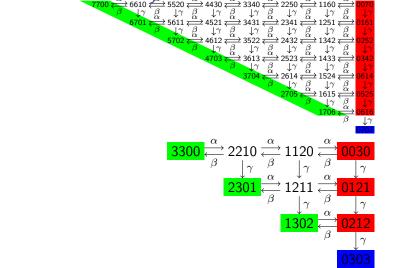
- CADP: current action decomposition property
 - ▶ $(P_1 \bowtie Q_1, P_2 \bowtie Q_2) \in \mathcal{H}$ and derivatives of same model then $(P_1, P_2) \in \mathcal{H}, (Q_1, Q_2) \in \mathcal{H}$
- ▶ if $P_1 \simeq P_2$, $Q_1 \simeq Q_2$ and $P_1 \bowtie_{L} Q_1$ has CADP and $P_2 \bowtie_{L} Q_2$ has CADP then $P_1 \bowtie_{L} Q_1 \simeq P_2 \bowtie_{L} Q_2$
 - ► $(P_1, P_2) \in \mathcal{H}$ then $(P_1 \Join_{L} Q, P_2 \Join_{L} Q) \in \mathcal{H}$
 - construct a suitable bisimulation over equivalence classes

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 - ▶ $(P_1 \bowtie Q_1, P_2 \bowtie Q_2) \in \mathcal{H}$ and derivatives of same model then $(P_1, P_2) \in \mathcal{H}, (Q_1, Q_2) \in \mathcal{H}$
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►
$$(P_1, P_2) \in \mathcal{H}$$
 then $(P_1 \Join_{\iota} Q, P_2 \Join_{\iota} Q) \in \mathcal{H}$

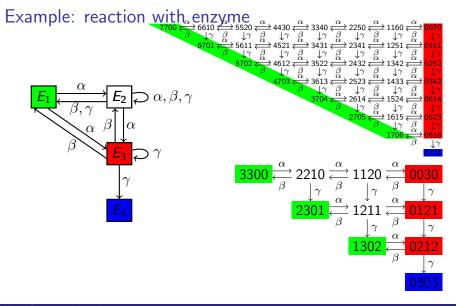
- construct a suitable bisimulation over equivalence classes
- For a well-defined Bio-PEPA system, Pⁿ ≏ P^m if they both have CADP and n, m ≥ k_↓ + max{k_↓, k_↑} + k_↑

Example: reaction with enzyme



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Thank you

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