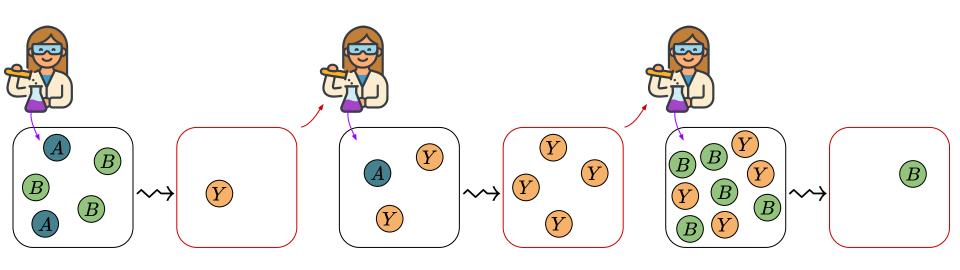
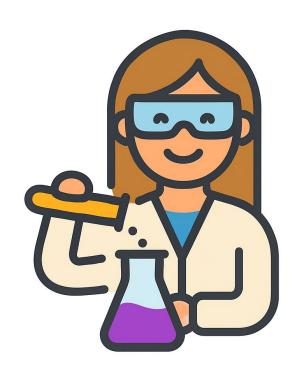
## Polynomial Simulation of CRN Models with Trimolecular Void Step-Cycle CRNs

The 22nd International Conference on Unconventional Computation and Natural Computation Sept 1-5, 2025 | Nice, France



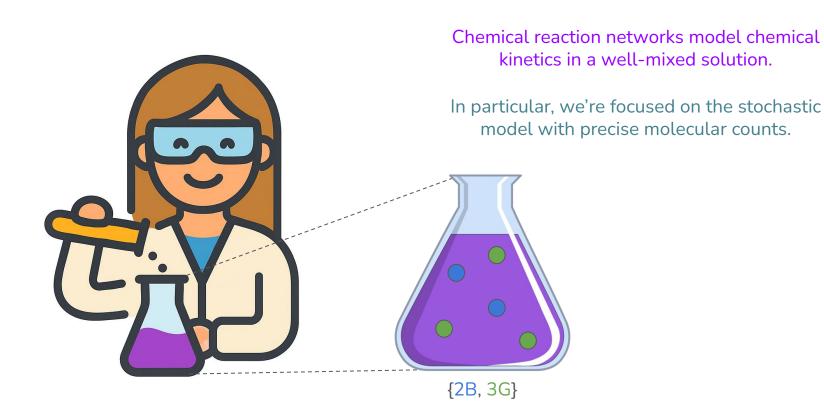
Austin Luchsinger, Aiden Massie, Robert Schweller, Evan Tomai, Tim Wylie

#### (Stochastic) Chemical Reaction Networks

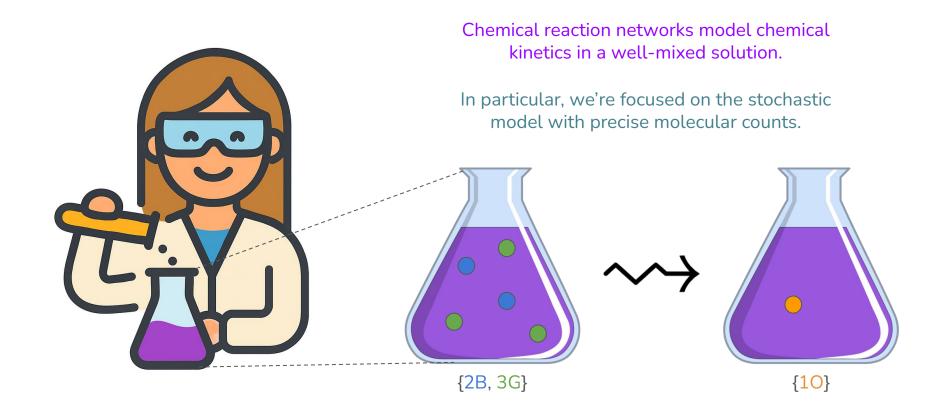


Chemical reaction networks model chemical kinetics in a well-mixed solution.

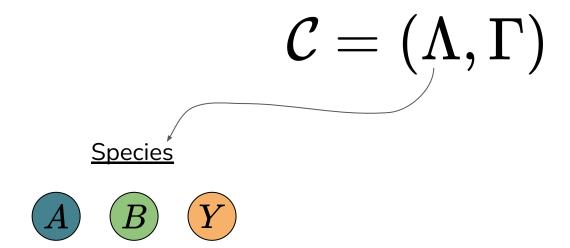
#### (Stochastic) Chemical Reaction Networks

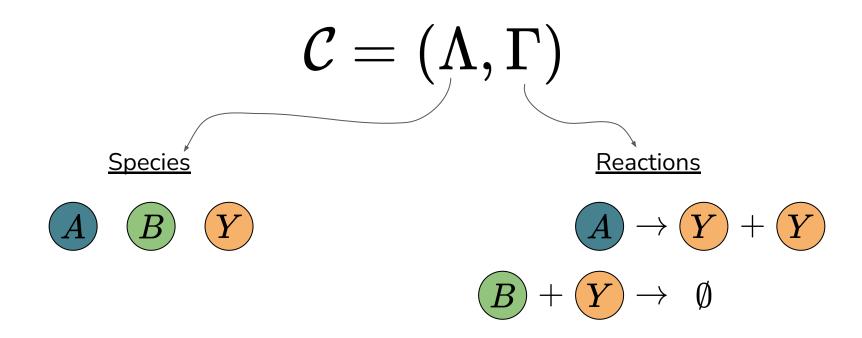


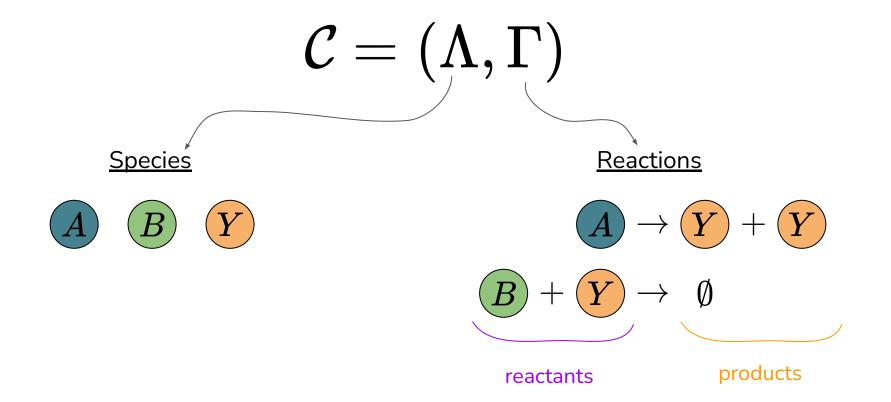
#### (Stochastic) Chemical Reaction Networks



$$\mathcal{C}=(\Lambda,\Gamma)$$

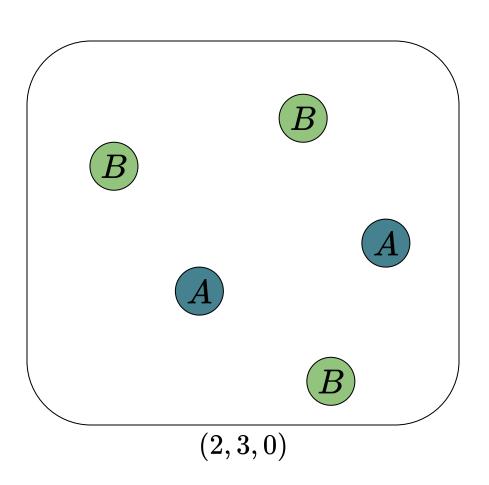






#### **CRN Configurations**

$$(a,b,y) \in \mathbb{Z}_{\geq 0}^{\Lambda}$$

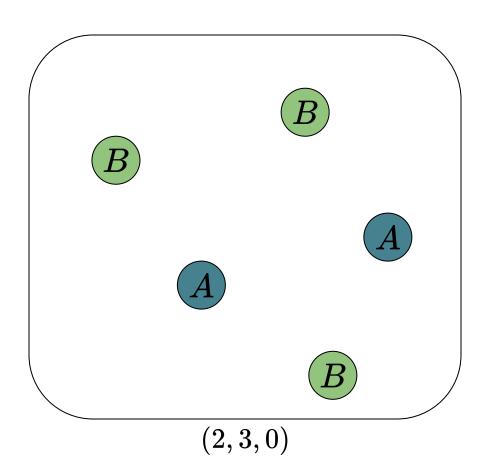


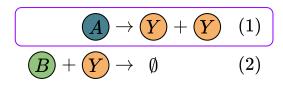
#### **CRN Configurations**

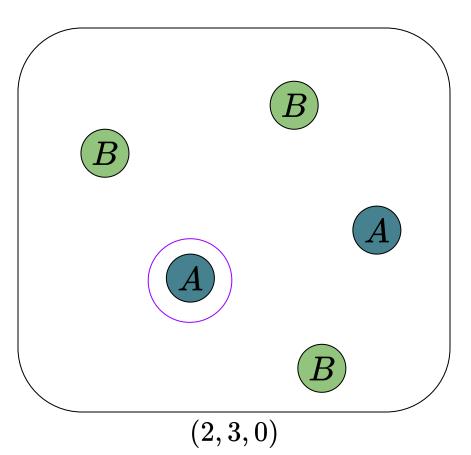
$$(a,b,y) \in \mathbb{Z}_{\geq 0}^{\Lambda}$$

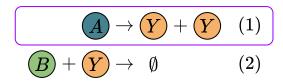
$$A \rightarrow Y + Y$$
 (1)

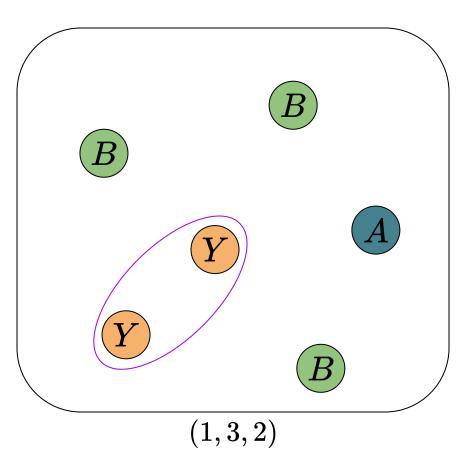
$$\bigcirc B + \bigcirc Y \rightarrow \emptyset$$
 (2)

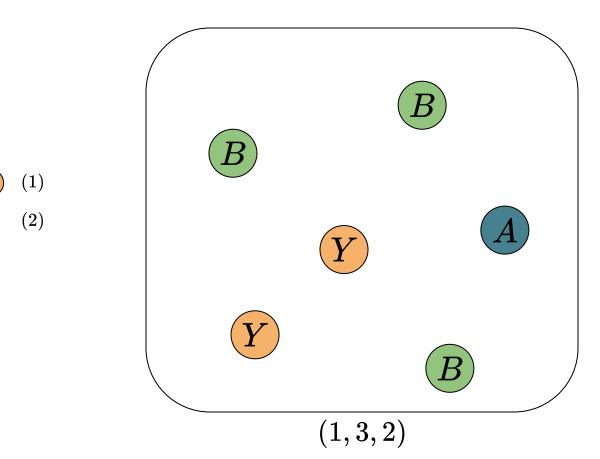


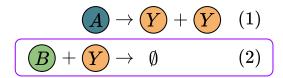


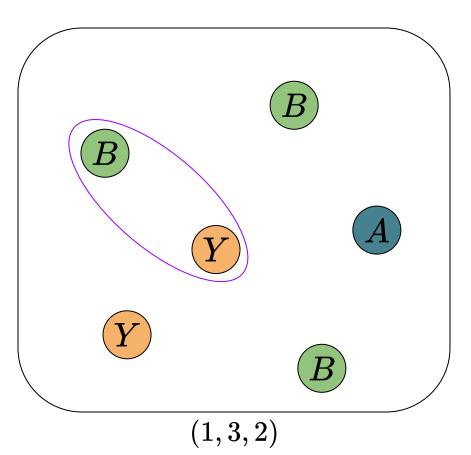


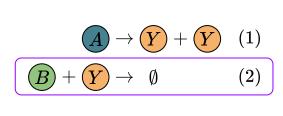


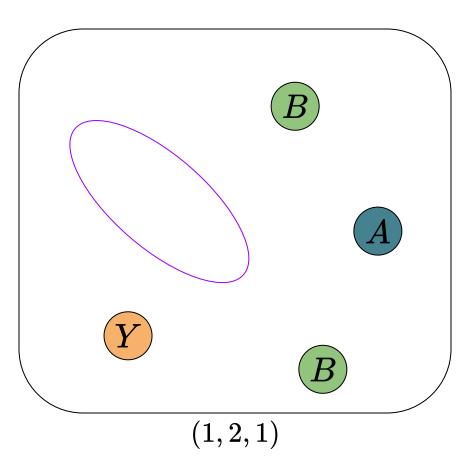


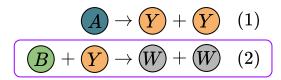


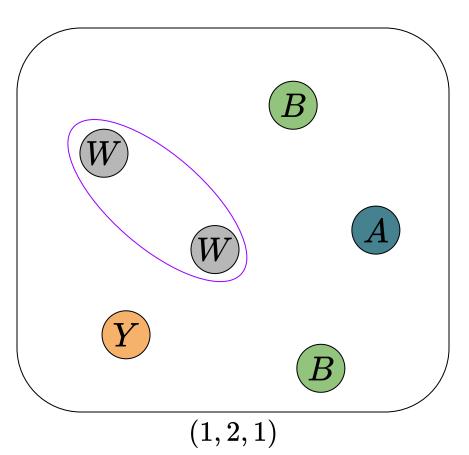


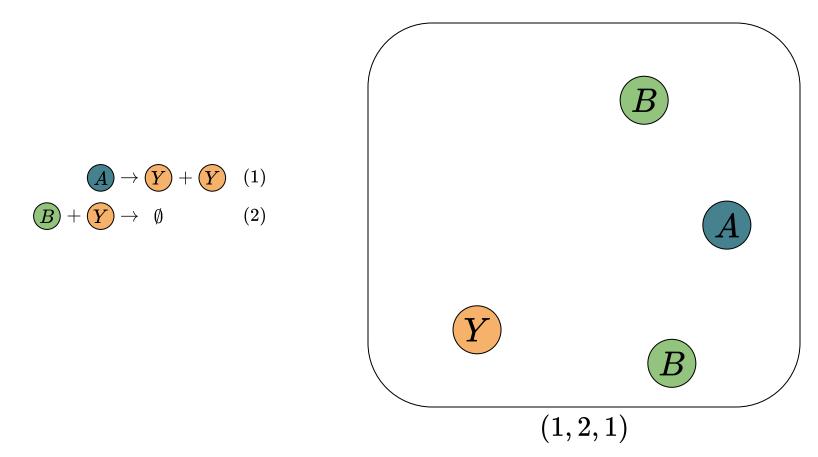


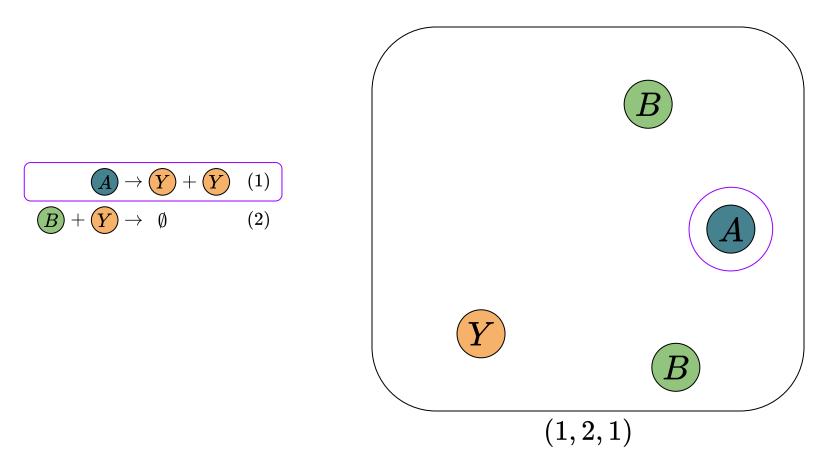


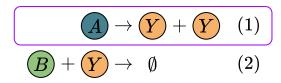


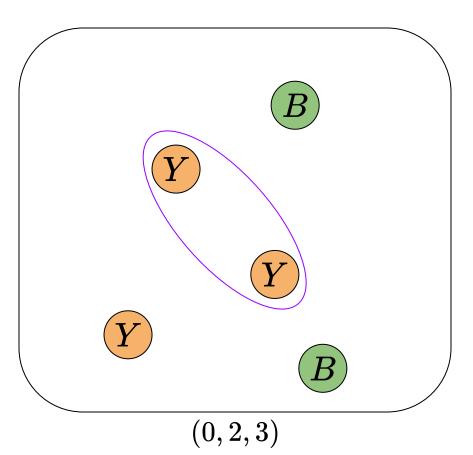


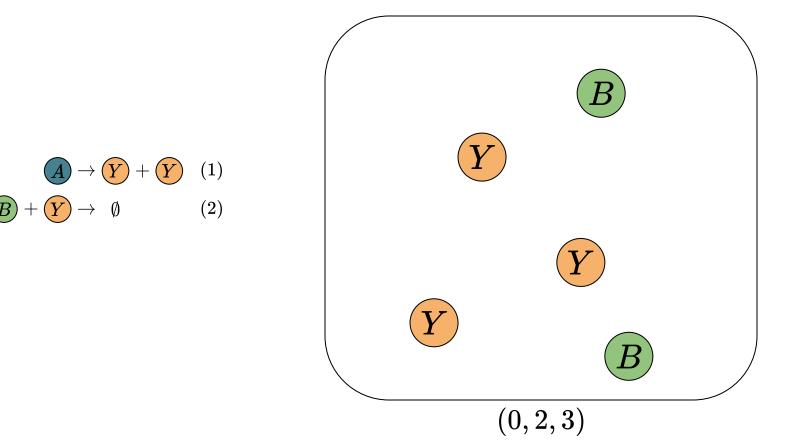


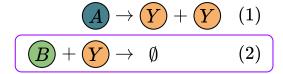


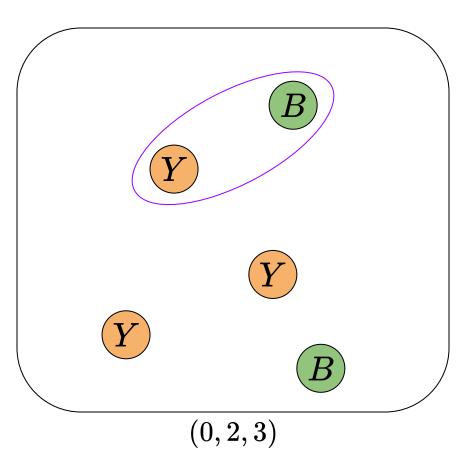


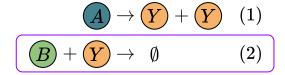


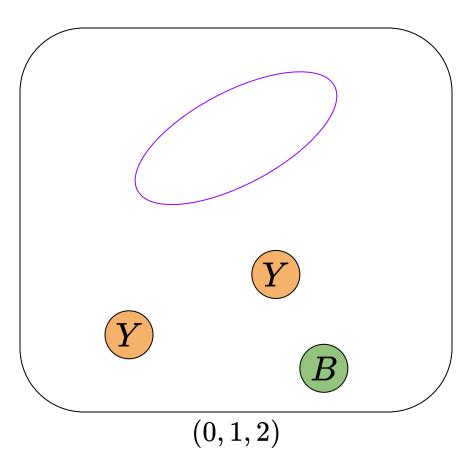


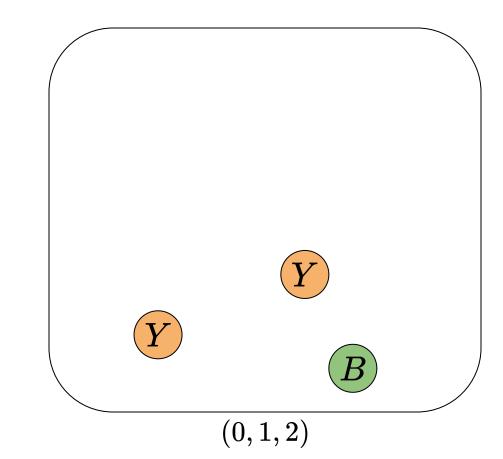


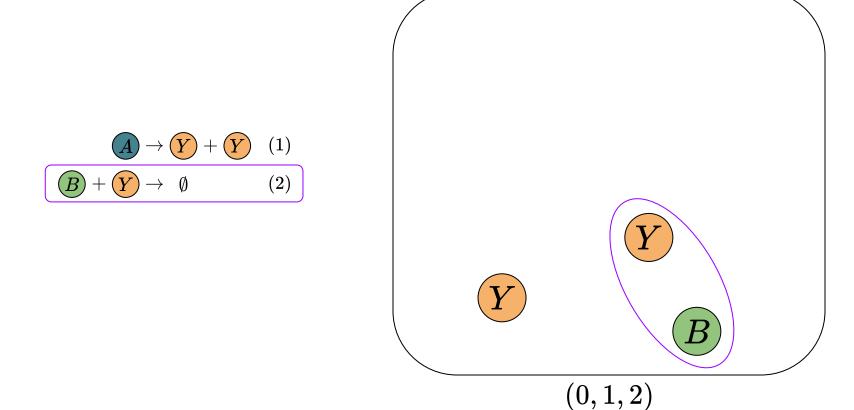


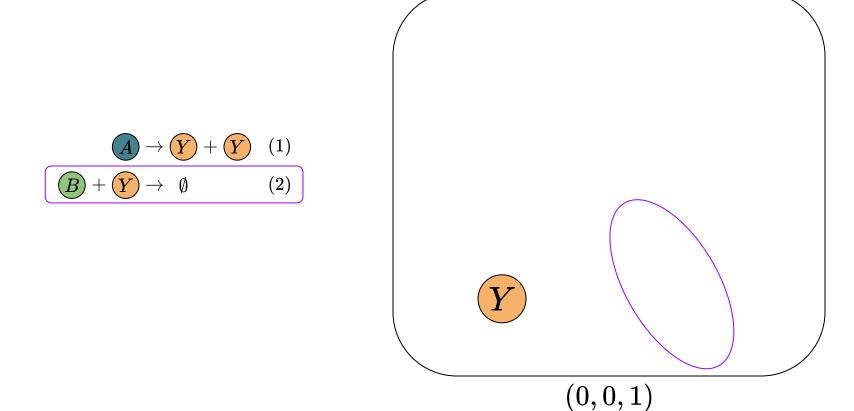


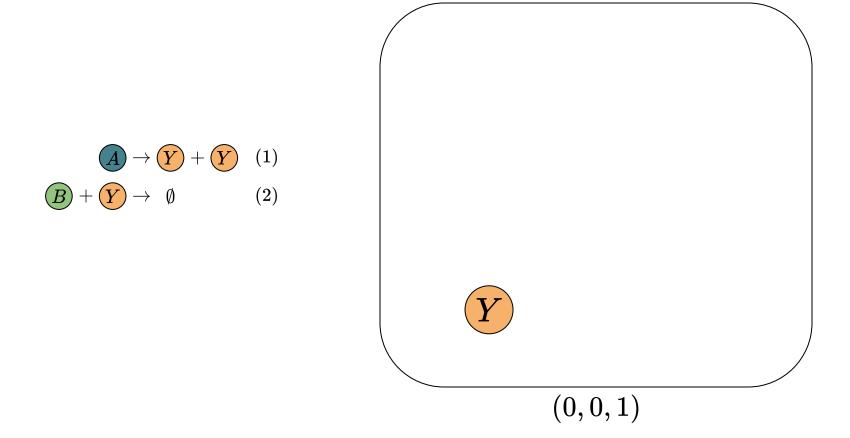












 $\{1Y\}$  is **terminal** since no reactions can happen (are applicable).

$$A \rightarrow Y + Y$$
 (1)

$$(B) + (Y) \rightarrow \emptyset$$
 (2)



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 $\{1Y\}$  is **reachable** from  $\{2A,3B\}$ 



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 $\{1Y\}$  is **reachable** from  $\{2A,3B\}$ 

$$\{2A, 3B\} \longrightarrow \{1Y\}$$



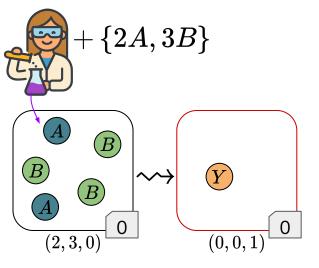
**Reactions** 





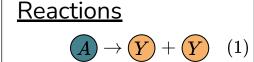


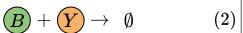


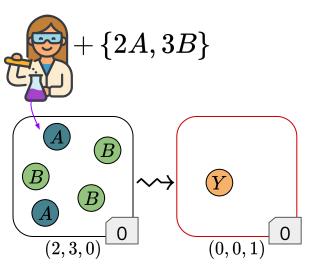


Step CRNs also specify a sequence of k steps that each add a collection of species to terminal configurations.

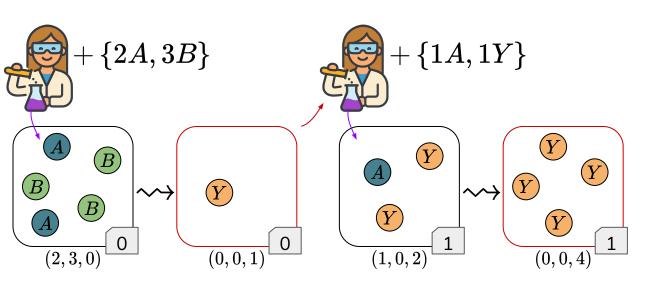








Step CRNs also specify a sequence of k steps that each add a collection of species to terminal configurations.



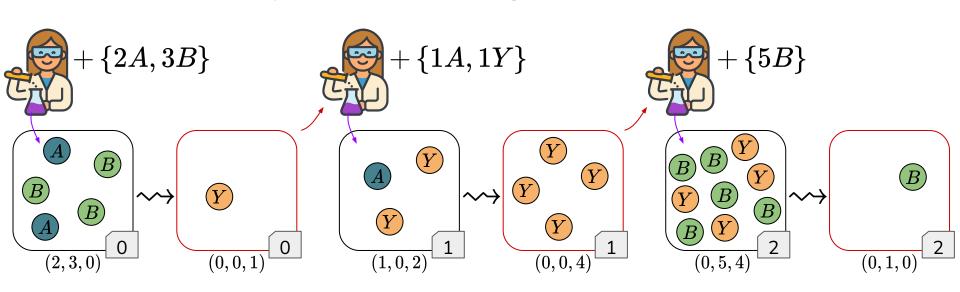
#### **Reactions**



$$(2)$$
  $(3)$   $(4)$ 

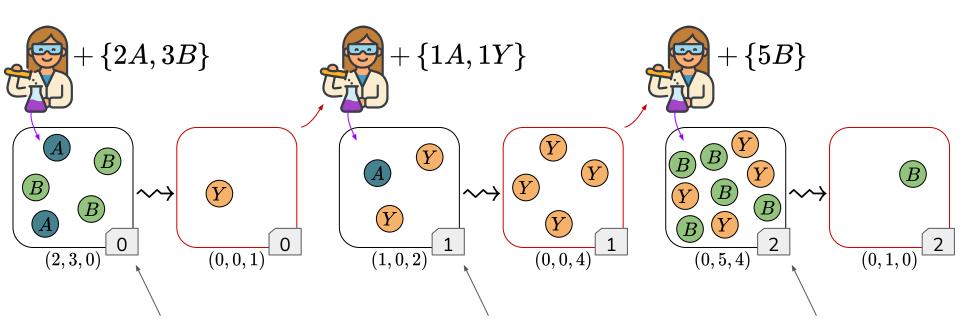
Step CRNs also specify a sequence of k steps that each add a collection of species to terminal configurations.

Reactions  $A \rightarrow Y + Y \qquad (1)$   $R \rightarrow Q \qquad (2)$ 

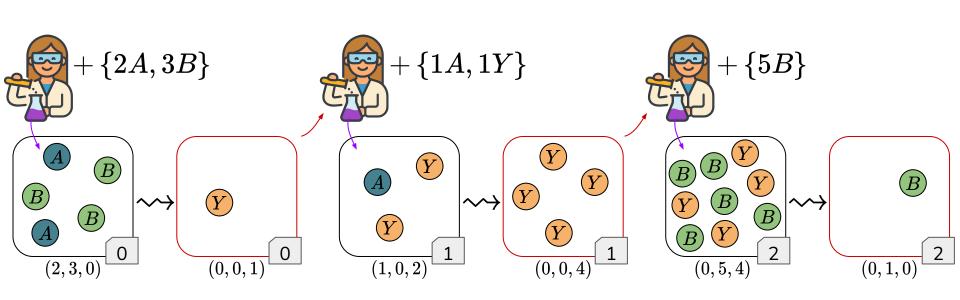


Step CRNs also specify a sequence of k steps that each add a collection of species to terminal configurations.

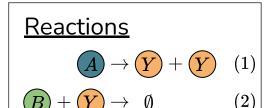
Reactions  $A \rightarrow Y + Y \qquad (1)$   $R + Y \rightarrow \emptyset \qquad (2)$ 

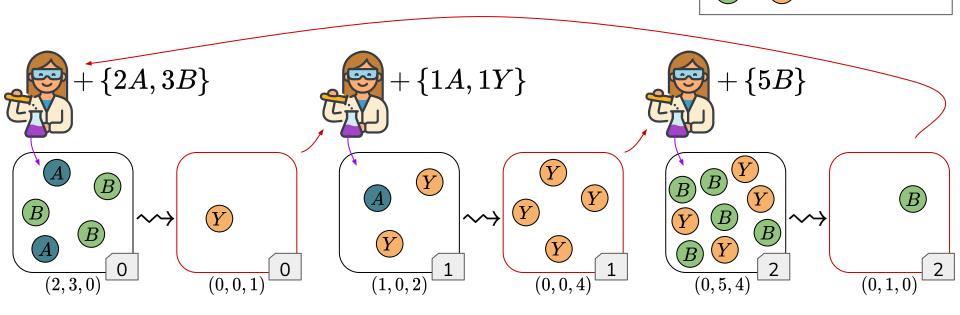


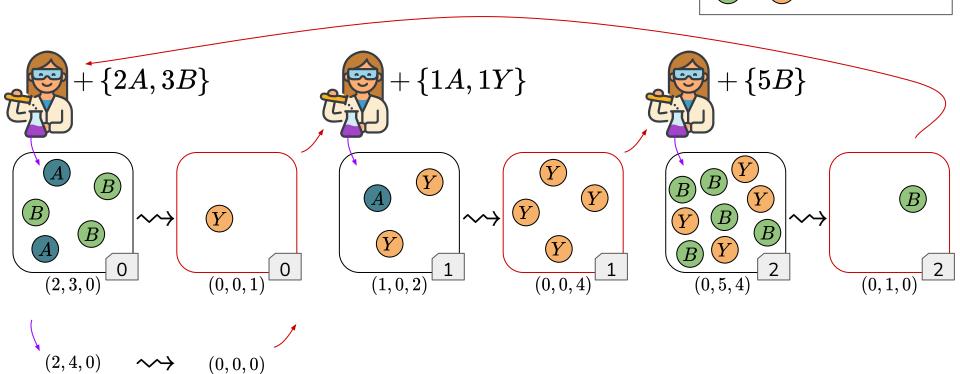
Step CRN Configurations also include an index to indicate the current step.

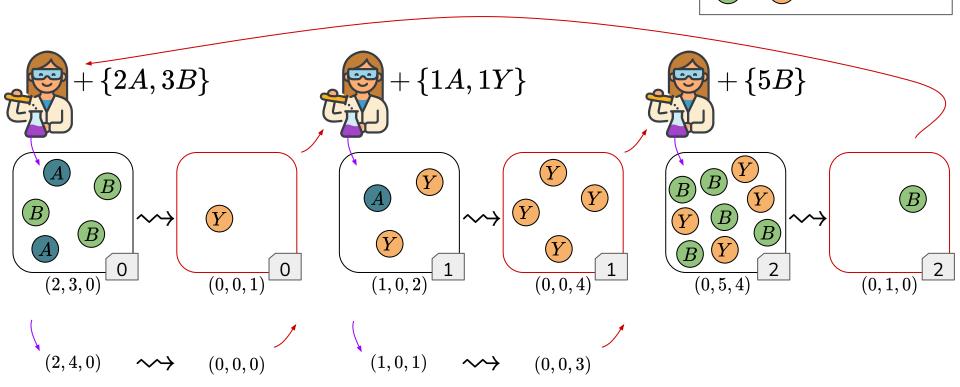


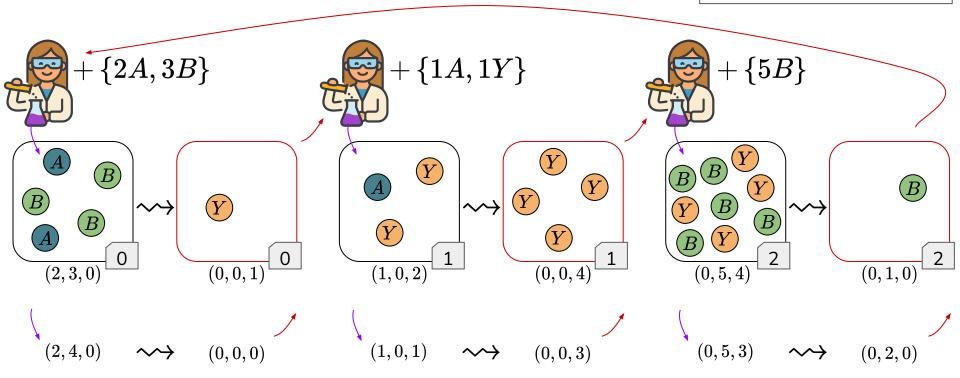
# Step CRN Configurations & Dynamics Step-Cycle



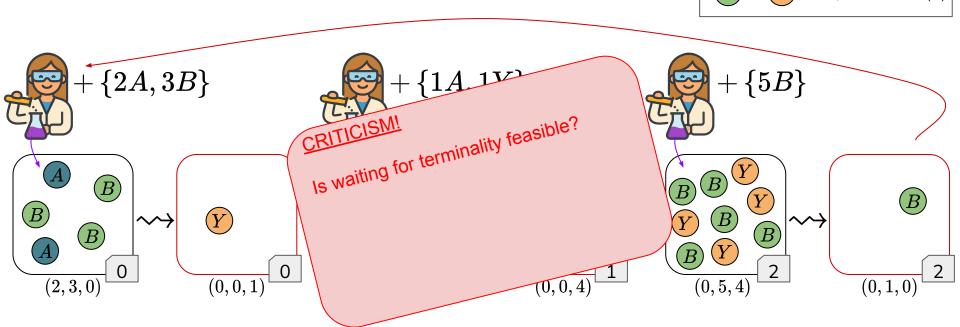


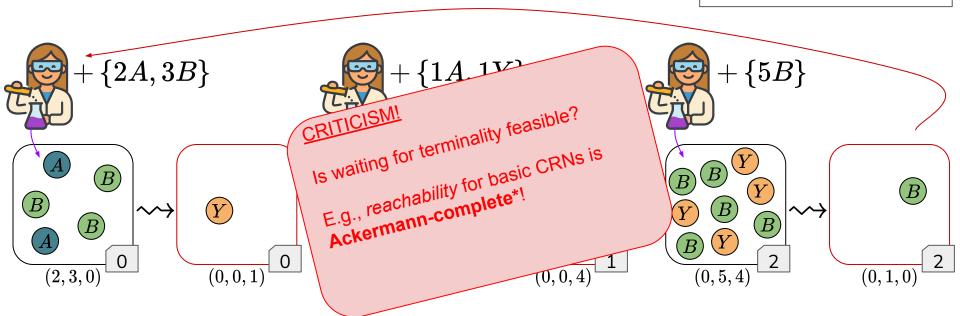






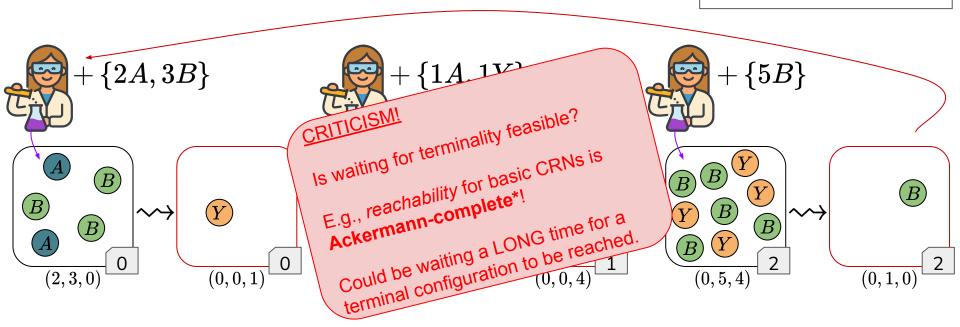
Reactions  $A \rightarrow Y + Y \qquad (1)$ 





<sup>\*[</sup>Wojciech Czerwiński and Łukasz Orlikowski, FOCS'21]

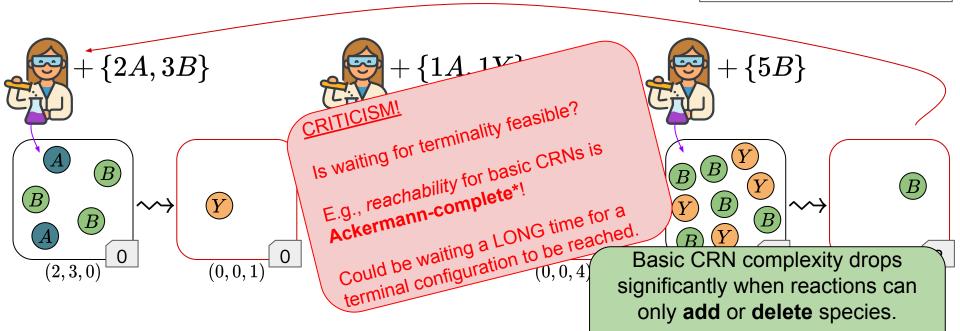
<sup>\*[</sup>Jérôme Leroux, FOCS'21]



<sup>\*[</sup>Wojciech Czerwiński and Łukasz Orlikowski, FOCS'21]

<sup>\*[</sup>Jérôme Leroux, FOCS'21]

**Reactions** 



\*[Wojciech Czerwiński and Łukasz Orlikowski, FOCS'21]

E.g., reachability falls within NP!

\*[Jérôme Leroux, FOCS'21]

#### Rule Size:

$$(2,0) A + B \rightarrow \emptyset$$

$$(3,0) \quad \boxed{A} + \boxed{B} + \boxed{Y} \rightarrow \emptyset$$

#### Rule Size:

$$(2,0) A + B \rightarrow \emptyset$$

$$(3.0) \quad A + B + Y \rightarrow \emptyset$$

$$(2,1) A + B \rightarrow A$$

$$(3,1) \quad A + B + Y \rightarrow B$$

$$(3,2) \quad A + B + Y \rightarrow A + B$$

Catalytic Reactions

#### Rule Size:

$$(2,0) \qquad \qquad A + B \rightarrow \emptyset$$

$$(3,0) \quad A + B + Y \rightarrow \emptyset$$

$$(2,1) A + B \rightarrow A$$

$$(3,1) \quad \boxed{A} + \boxed{B} + \boxed{Y} \rightarrow \boxed{B}$$

$$(3,2) \quad A + B + Y \rightarrow A + B$$

We consider Step-Cycle CRNs that use only (3,1) void rules.

Catalytic Reactions

#### Rule Size:

$$(2,0) \qquad \qquad A + B \rightarrow \emptyset$$

$$(3,0) \quad A + B + Y \rightarrow \emptyset$$

$$(2,1) A + B \rightarrow A$$

$$(3,1) \quad A + B + Y \rightarrow B$$

$$(3,2) \quad A + B + Y \rightarrow A + B$$

We consider Step-Cycle CRNs that use only (3,1) void rules.

Despite the significant loss in power for basic CRNs, (3,1) Void Step-Cycle CRNs are *equivalent* to general Step-Cycle CRNs!

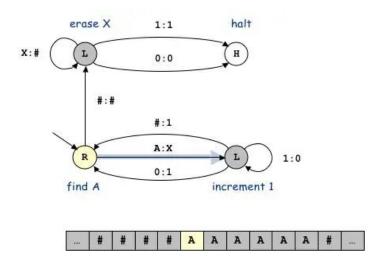
Catalytic Reactions

Register Machine

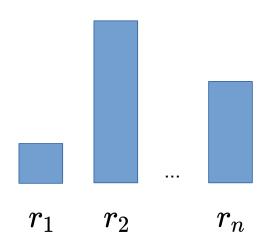
**Turing Machine** 

Register Machine

#### **Turing Machine**

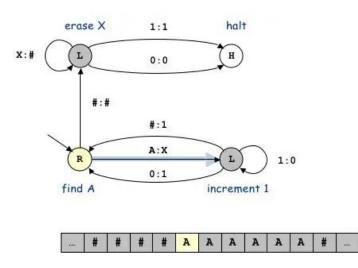


#### Register Machine



$$inc(r_i,s_j) \ dec(r_i,s_j,s_k)$$

#### **Turing Machine**



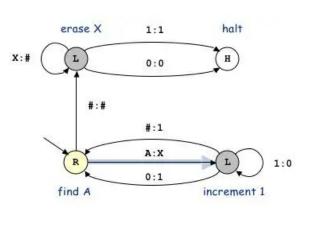
Register Machine

 $r_1 \qquad r_2 \qquad \qquad r$ 

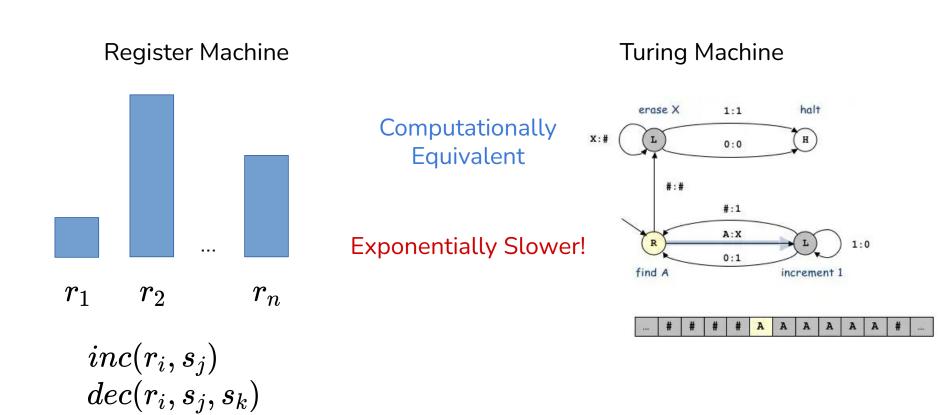
 $inc(r_i,s_j) \ dec(r_i,s_j,s_k)$ 

Computationally Equivalent

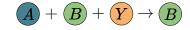
#### **Turing Machine**



AAAAAA



(3,1) Void Step-Cycle CRN  $C^\prime$ 

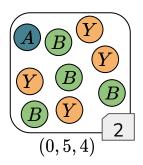


General Step-Cycle CRN  $\,C\,$ 

$$D + A \rightarrow B + Y + C$$

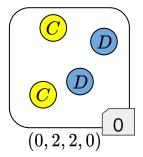
(3,1) Void Step-Cycle CRN  $C^\prime$ 





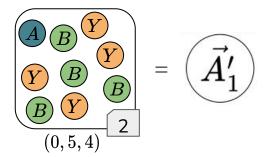
General Step-Cycle CRN  $\,C\,$ 

$$D + A \rightarrow B + Y + C$$



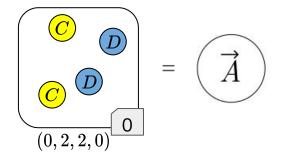
(3,1) Void Step-Cycle CRN  $C^\prime$ 

$$A + B + Y \rightarrow B$$



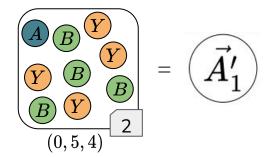
General Step-Cycle CRN  $\,C\,$ 

$$D + A \rightarrow B + Y + C$$



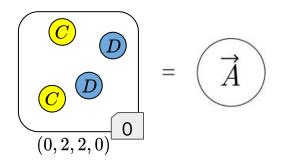
(3,1) Void Step-Cycle CRN  $C^\prime$ 

$$A + B + Y \rightarrow B$$



General Step-Cycle CRN  $\,C\,$ 

$$D + A \rightarrow B + Y + C$$



Polynomial-time computable function  $\,M: \mathrm{configs}_{C'} o \mathrm{configs}_{C} \,$ 

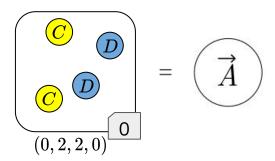
(3,1) Void Step-Cycle CRN  $C^\prime$ 

$$A + B + Y \rightarrow B$$

 $M\left(\overrightarrow{A_1'}\right) \,=\, \overrightarrow{A}$ 

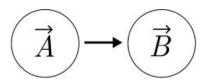
General Step-Cycle CRN  $\,C\,$ 

$$D + A \rightarrow B + Y + C$$



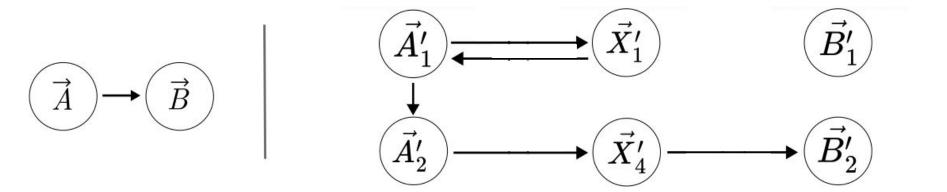
Polynomial-time computable function  $M: \mathrm{configs}_{C'} o \mathrm{configs}_{C}$ 

Configuration Space of Original System



Configuration Space of Original System

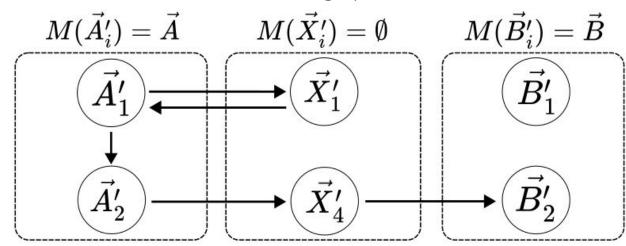
Configuration Space of Simulating System



Configuration Space of Original System

 $\rightarrow (\overrightarrow{B})$ 

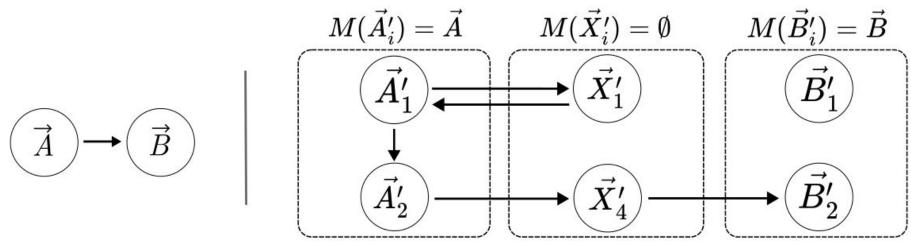
Configuration Space of Simulating System



 $M: \operatorname{configs}_{C'} o \operatorname{configs}_C$ 

Configuration Space of Original System

Configuration Space of Simulating System

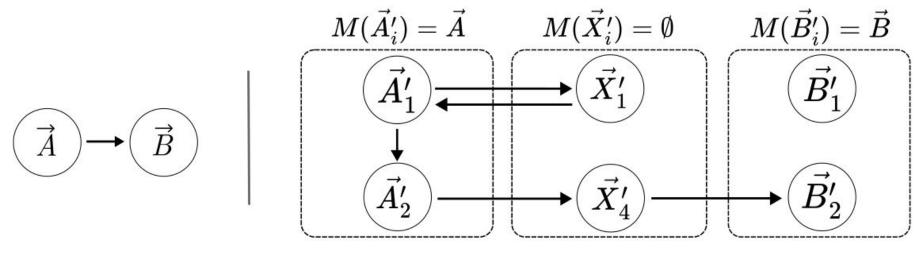


 $M: \operatorname{configs}_{C'} o \operatorname{configs}_C$ 

**Definition 7 (It Follows).** We say system T follows system T' if whenever  $\overrightarrow{A'} \Rightarrow_{T'} \overrightarrow{B'}$  and  $M(\overrightarrow{A'}) \neq M(\overrightarrow{B'})$ , then  $M(\overrightarrow{A'}) \rightarrow_T M(\overrightarrow{B'})$ .

Configuration Space of Original System

Configuration Space of Simulating System



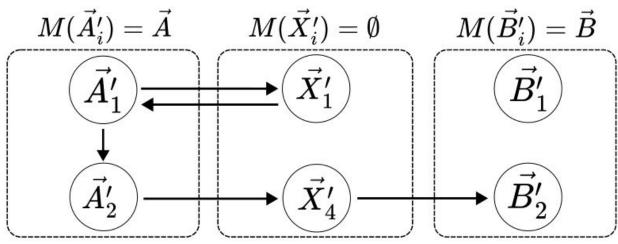
 $M: \operatorname{configs}_{C'} o \operatorname{configs}_C$ 

**Definition 8 (Models).** We say system T' models system T if  $\overrightarrow{A} \to_T \overrightarrow{B}$  implies that  $\forall \overrightarrow{A'} \in [\![\overrightarrow{A}]\!]$ ,  $\exists \overrightarrow{B'} \in [\![\overrightarrow{B}]\!]$  such that  $\overrightarrow{A'} \Rightarrow_{T'} \overrightarrow{B'}$ .

Configuration Space of Original System

 $\overrightarrow{A}$   $\longrightarrow$   $\overrightarrow{B}$ 

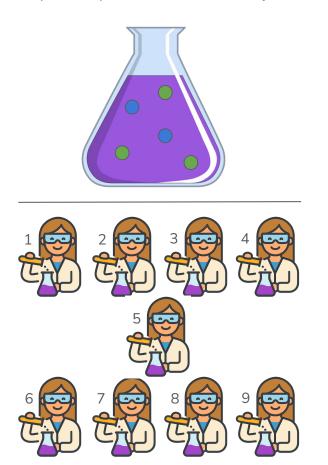
Configuration Space of Simulating System



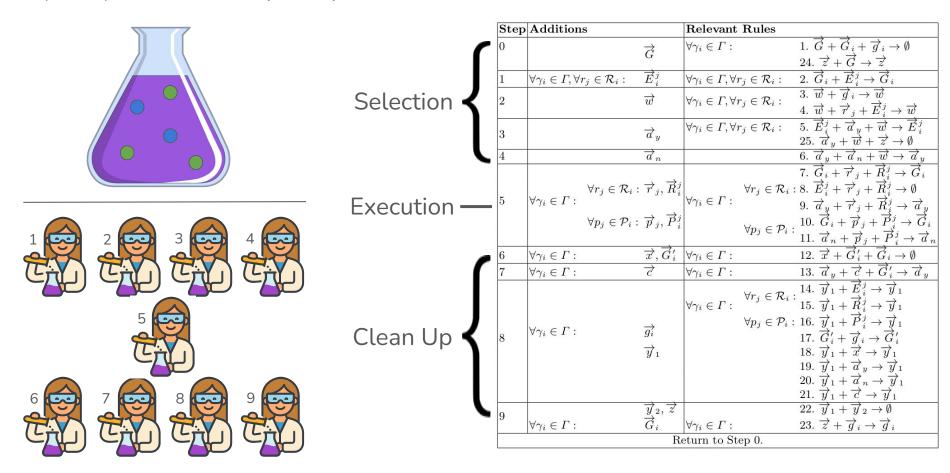
 $M: \operatorname{configs}_{C'} o \operatorname{configs}_C$ 

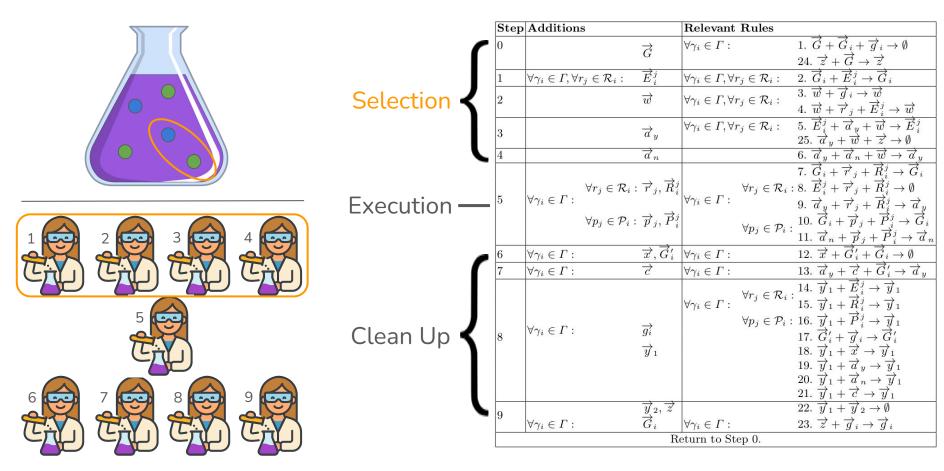
- Polynomial Simulation:
- Polynomial System Size
- (Expected) Polynomial System Transitions

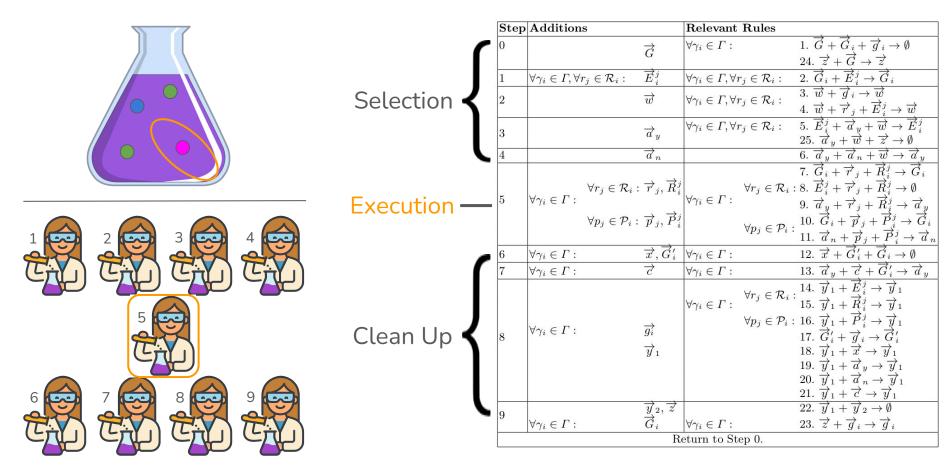
Step	Addition	s		Relevant Rules						
0			$\overrightarrow{G}$	$\forall \gamma_i \in \mathcal{A}$	$\Gamma$ :		$1. \overrightarrow{G} + \overrightarrow{G}_i + \overrightarrow{g}_i \to \emptyset$			
							$24. \ \overrightarrow{z} + \overrightarrow{G} \rightarrow \overrightarrow{z}$			
1	$\forall \gamma_i \in \varGamma, \forall i$	$r_j \in \mathcal{R}_i$ :	$\overrightarrow{E}_{i}^{j}$	$\forall \gamma_i \in \mathcal{A}$	$\Gamma, \forall r$	$j \in \mathcal{R}_i$ :	$2. \ \overrightarrow{G}_i + \overrightarrow{E}_i^j \to \overrightarrow{G}_i$			
2			$\overrightarrow{w}$	$\forall \gamma_i \in$	$\Gamma, \forall r$	$j \in \mathcal{R}_i$ :	$3. \ \overrightarrow{w} + \overrightarrow{g}_i \rightarrow \overrightarrow{w}$			
50.0				10 100		TS:	$4. \ \overrightarrow{w} + \overrightarrow{r}_j + \overrightarrow{E}_i^j \to \overrightarrow{w}$			
3			$\overrightarrow{a}_y$	$\forall \gamma_i \in \mathcal{A}$	$\Gamma, \forall r$	$j \in \mathcal{R}_i$ :	$ \begin{array}{ccc} 5. \overrightarrow{E}_{i}^{j} + \overrightarrow{a}_{y} + \overrightarrow{w} \rightarrow \overrightarrow{E}_{i}^{j} \\ 25. \overrightarrow{a}_{y} + \overrightarrow{w} + \overrightarrow{z} \rightarrow \emptyset \end{array} $			
			1570				$25. \ \alpha_y + w + z \to \emptyset$			
4			$\overrightarrow{a}_n$				$6. \overrightarrow{a}_y + \overrightarrow{a}_n + \overrightarrow{w} \to \overrightarrow{a}_y$			
	$\forall \gamma_i \in \varGamma :$	$\forall r_j \in \mathcal{R}_i$ :	$\overrightarrow{r}_j, \overrightarrow{R}_i^j$				7. $\overrightarrow{G}_i + \overrightarrow{r}_j + \overrightarrow{R}_i^j \rightarrow \overrightarrow{G}_i$			
(3)				$\forall \gamma_i \in I$		$\forall r_j \in \mathcal{R}_i$ :	$: 8. \ \overrightarrow{E}_{i}^{j} + \overrightarrow{r}_{j} + \overrightarrow{R}_{i}^{j} \to \emptyset $			
5					$\Gamma$ :		9. $\overrightarrow{a}_y + \overrightarrow{r}_j + \overrightarrow{R}_i^j \rightarrow \overrightarrow{a}_y$			
		$\forall p_j \in \mathcal{P}_i$ :	$\overrightarrow{p}_i, \overrightarrow{P}_i^j$			V - 0	9. $a_y + r_j + R_i \rightarrow a_y$ 10. $\overrightarrow{G}_i + \overrightarrow{p}_j + \overrightarrow{P}_i^j \rightarrow \overrightarrow{G}_i$			
						$\forall p_j \in \mathcal{P}_i$	$11. \overrightarrow{a}_n + \overrightarrow{p}_j + \overrightarrow{P}_i^j \rightarrow \overrightarrow{a}_n$			
6	$\forall \gamma_i \in \Gamma$ :		$\overrightarrow{x}, \overrightarrow{G}'_i$	$\forall \gamma_i \in \mathcal{A}$	$\Gamma$ :		12. $\overrightarrow{x} + \overrightarrow{G}'_i + \overrightarrow{G}_i \to \emptyset$			
7	$\forall \gamma_i \in \Gamma$ :		$\overrightarrow{c}$	$\forall \gamma_i \in \mathcal{A}$	$\Gamma$ :		13. $\overrightarrow{a}_y + \overrightarrow{c} + \overrightarrow{G}'_i \rightarrow \overrightarrow{a}_y$			
						V	$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$			
	$\forall \gamma_i \in \Gamma :$		$\overrightarrow{g_i}$ $\overrightarrow{y}_1$	$\forall \gamma_i \in I$	$\Gamma$ :	$\forall r_j \in \mathcal{R}_i$ :	$15. \overrightarrow{y}_1 + \overrightarrow{R}_i^j \rightarrow \overrightarrow{y}_1$			
				00.000000000000000000000000000000000000		$\forall p_i \in \mathcal{P}_i$	$: 16. \overrightarrow{y}_1 + \overrightarrow{P}_i^j \to \overrightarrow{y}_1$			
8						- 3	17. $\overrightarrow{G}'_i + \overrightarrow{g}_i \rightarrow \overrightarrow{G}'_i$			
							18. $\overrightarrow{y}_1 + \overrightarrow{x} \rightarrow \overrightarrow{y}_1$			
			0 1				19. $\overrightarrow{y}_1 + \overrightarrow{a}_y \rightarrow \overrightarrow{y}_1$			
							$20. \ \overrightarrow{y}_1 + \overrightarrow{a}_n \to \overrightarrow{y}_1$			
							21. $\overrightarrow{y}_1 + \overrightarrow{c} \rightarrow \overrightarrow{y}_1$			
9			$\overrightarrow{y}_2, \overrightarrow{z}$ $\overrightarrow{G}_i$				$22. \ \overrightarrow{y}_1 + \overrightarrow{y}_2 \to \emptyset$			
9	$\forall \gamma_i \in \Gamma$ :		$\overrightarrow{G}_i$	$\forall \gamma_i \in \mathcal{A}$	$\Gamma$ :		$23. \ \overrightarrow{z} + \overrightarrow{g}_i \to \overrightarrow{g}_i$			
Return to Step 0.										

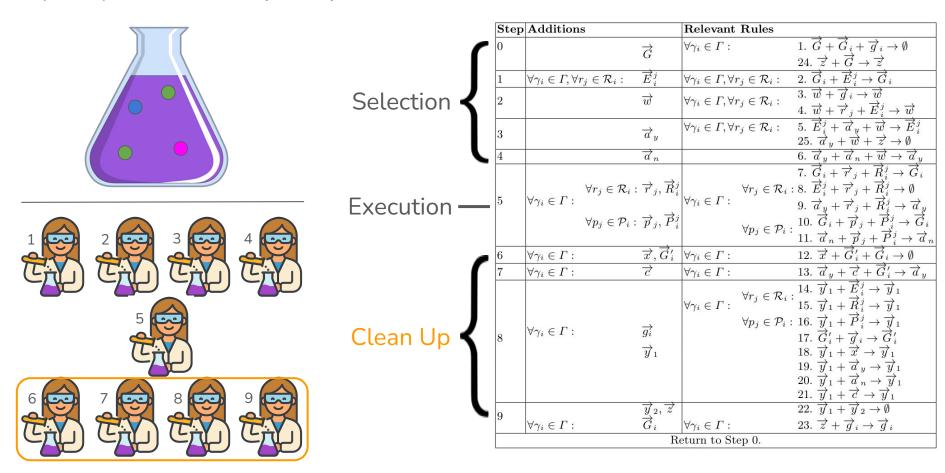


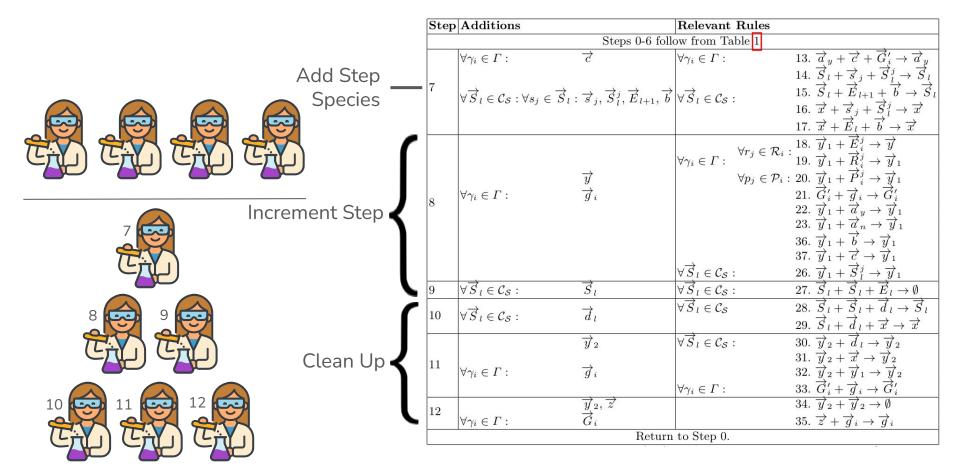
Step	ep Additions			Relevant Rules				
0			$\overrightarrow{G}$	$\forall \gamma_i \in \Gamma$ :		$1. \overrightarrow{G} + \overrightarrow{G}_i + \overrightarrow{g}_i \to \emptyset$		
						$24. \ \overrightarrow{z} + \overrightarrow{G} \rightarrow \overrightarrow{z}$		
1	$\forall \gamma_i \in \varGamma, \forall$	$r_j \in \mathcal{R}_i$ :	$\overrightarrow{E}_{i}^{j}$	$\forall \gamma_i \in \Gamma, \forall$	$r_j \in \mathcal{R}_i$ :	$2. \ \overrightarrow{G}_i + \overrightarrow{E}_i^j \to \overrightarrow{G}_i$		
2			$\overrightarrow{w}$	$\forall \gamma_i \in \Gamma, \forall$	$r_j \in \mathcal{R}_i$ :	$3. \overrightarrow{w} + \overrightarrow{g}_i \to \overrightarrow{w}$		
				\ - T\	· - D	$\underbrace{4. \overrightarrow{w} + \overrightarrow{r}_j + \overrightarrow{E}_i^j \rightarrow \overrightarrow{w}}_{z \rightarrow i}$		
3			$\overrightarrow{a}_y$	$\forall \gamma_i \in \Gamma, \forall$	$r_j \in \mathcal{R}_i$ :	5. $\overrightarrow{E}_{i}^{j} + \overrightarrow{a}_{y} + \overrightarrow{w} \rightarrow \overrightarrow{E}_{i}^{j}$ 25. $\overrightarrow{a}_{y} + \overrightarrow{w} + \overrightarrow{z} \rightarrow \emptyset$		
4			$\overrightarrow{a}_n$			$6. \overrightarrow{a}_y + \overrightarrow{a}_n + \overrightarrow{w} \to \overrightarrow{a}_y$		
						7. $\overrightarrow{G}_i + \overrightarrow{r}_j + \overrightarrow{R}_i^j \rightarrow \overrightarrow{G}_i$		
					$\forall r_j \in \mathcal{R}_i$ :	$\begin{array}{l} 1. \ G_{i} + \overrightarrow{r}_{j} + \overrightarrow{R}_{i} \to G_{i} \\ 1. \ 8. \ \overrightarrow{E}_{i}^{j} + \overrightarrow{r}_{j} + \overrightarrow{R}_{i}^{j} \to \emptyset \\ 1. \ 9. \ \overrightarrow{a}_{y} + \overrightarrow{r}_{i} + \overrightarrow{R}_{j}^{j} \to \overrightarrow{a}_{y} \end{array}$		
5	$\forall \gamma_i \in \varGamma :$					9. $\overrightarrow{a}_y + \overrightarrow{r}_j + \overrightarrow{R}_i^j \rightarrow \overrightarrow{a}_y$		
		$\forall p_j \in \mathcal{P}_i$ :	$\overrightarrow{p}_j, \overrightarrow{P}_i^j$		$\forall n \in \mathcal{D}_i$	$10. \overrightarrow{G}_i + \overrightarrow{p}_j + \overrightarrow{P}_i^j \rightarrow \overrightarrow{G}_i$		
					$VPj \subset Ii$ .	11. $a_n + p_j + P_i \rightarrow a_n$		
6	$\forall \gamma_i \in \Gamma$ :		$\overrightarrow{x}, \overrightarrow{G}'_i$	$\forall \gamma_i \in \Gamma$ :		12. $\overrightarrow{x} + \overrightarrow{G}'_i + \overrightarrow{G}_i \to \emptyset$		
7	$\forall \gamma_i \in \Gamma$ :		$\overrightarrow{c}$	$\forall \gamma_i \in \Gamma$ :		13. $\overrightarrow{a}_y + \overrightarrow{c} + \overrightarrow{G}'_i \rightarrow \overrightarrow{a}_y$		
					$\forall r_i \in \mathcal{R}_i$	$ \begin{array}{c}     14. \ \overrightarrow{y}_1 + \overrightarrow{E}_i^j \to \overrightarrow{y}_1 \\     15. \ \overrightarrow{y}_1 + \overrightarrow{R}_i^j \to \overrightarrow{y}_1 \end{array} $		
	$\forall \gamma_i \in \Gamma$ :			$\forall \gamma_i \in \Gamma$ :				
			$\overrightarrow{g_i}$ $\overrightarrow{y}_1$		$\forall p_j \in \mathcal{P}_i$ :	16. $\overrightarrow{y}_1 + \overrightarrow{P}_i^j \rightarrow \overrightarrow{y}_1$		
8	$\forall \gamma_i \in I$ :					17. $\overrightarrow{G}'_i + \overrightarrow{g}_i \rightarrow \overrightarrow{G}'_i$		
						18. $\overrightarrow{y}_1 + \overrightarrow{x} \rightarrow \overrightarrow{y}_1$		
						19. $\overrightarrow{y}_1 + \overrightarrow{a}_y \rightarrow \overrightarrow{y}_1$		
						20. $\overrightarrow{y}_1 + \overrightarrow{a}_n \rightarrow \overrightarrow{y}_1$		
			$\rightarrow$			$ \begin{array}{ccc} 21. \ \overrightarrow{y}_1 + \overrightarrow{c} \to \overrightarrow{y}_1 \\ 22. \ \overrightarrow{y}_1 + \overrightarrow{y}_2 \to \emptyset \end{array} $		
9	$\forall \alpha \in \Gamma$		$\overrightarrow{y}_2, \overrightarrow{z}$ $\overrightarrow{G}_i$	$\forall \gamma_i \in \Gamma$ :		22. $y_1 + y_2 \rightarrow y_1$ 23. $\overrightarrow{z} + \overrightarrow{g}_i \rightarrow \overrightarrow{g}_i$		
	$\forall \gamma_i \in \Gamma :$		200.00		ten ()	$20. \ z + y_i \rightarrow y_i$		
Return to Step 0.								

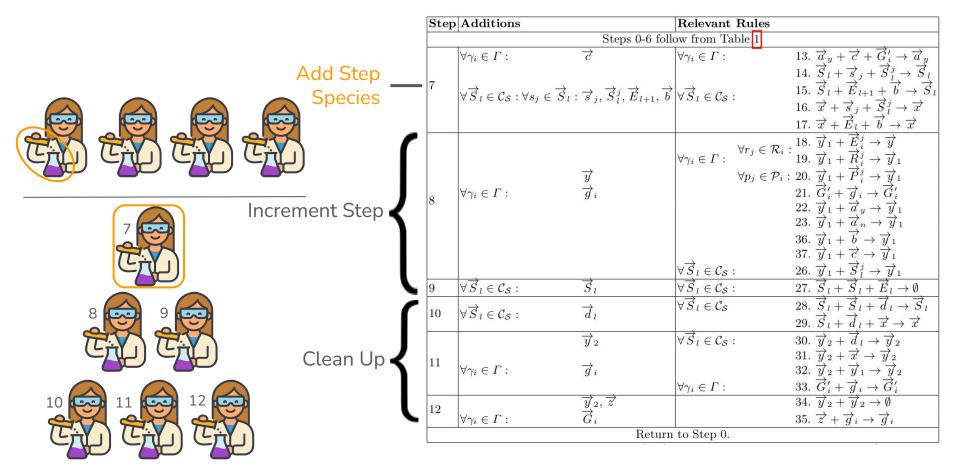


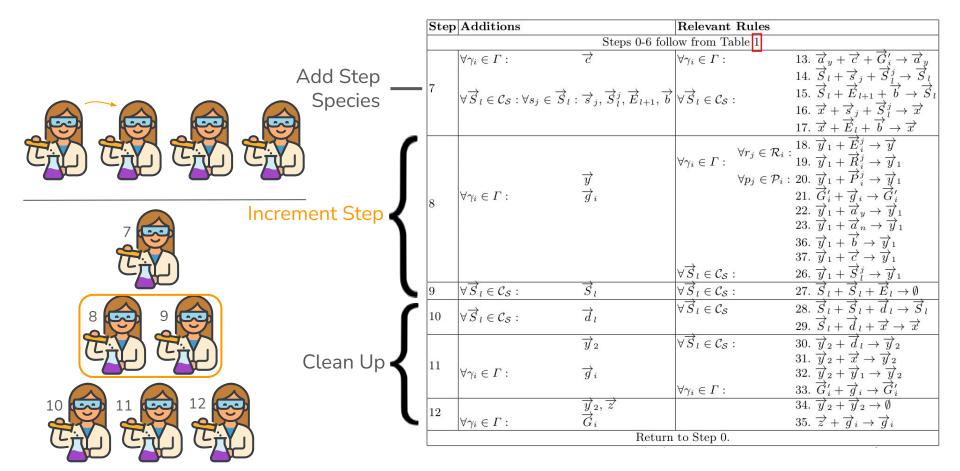


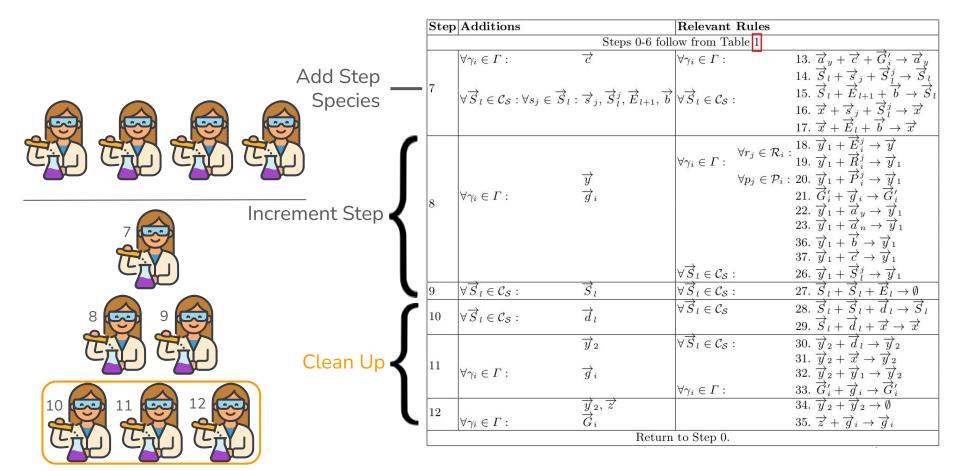


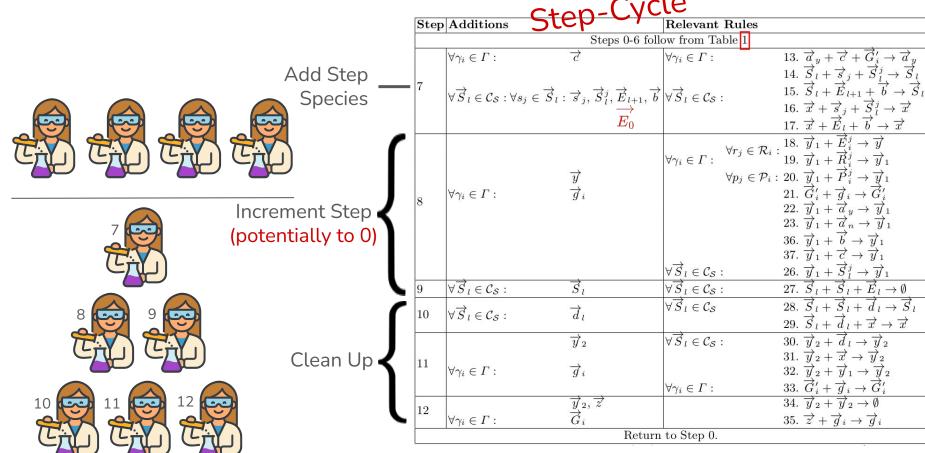












# (3,1) Step-Cycle CRNs is Turing Universal

(3,1) Void Step-Cycle CRN  $C^\prime$ 

General Step-Cycle CRN  $\,C\,$ 







equivalent under polynomial simulation

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(3,1) Void Step-Cycle CRN  $C^\prime$ 

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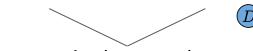
Step-Cycle CRNs are Turing-Universal\*

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(3,1) Void Step-Cycle CRN  $C^\prime$ 

General Step-Cycle CRN  $\,C\,$ 





 $D + A \rightarrow B + Y + C$ 

equivalent under polynomial simulation

(3,1) Void CRN

General CRN

Reachability is NP-complete

Reachability is
Ackermann-complete

#### **Future Work**

Our notion of polynomial simulation actually captures "expected" polynomial-ness. Can we achieve a tighter connection between the transition probabilities for both the original and simulating systems?

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Questions?