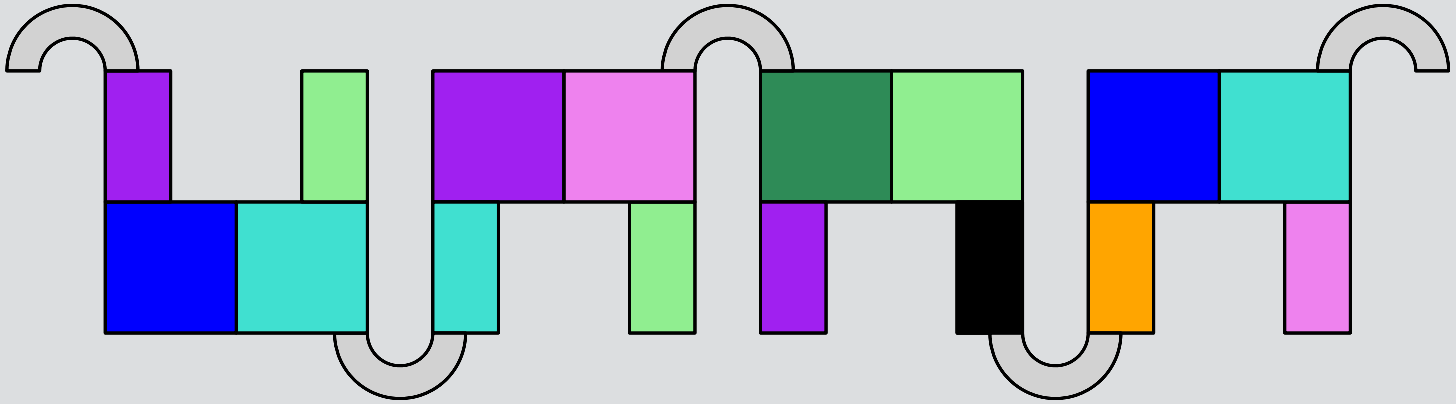
Non-Determinism Reduces Construction Time in Active Self-Assembly Using an Insertion Primitive



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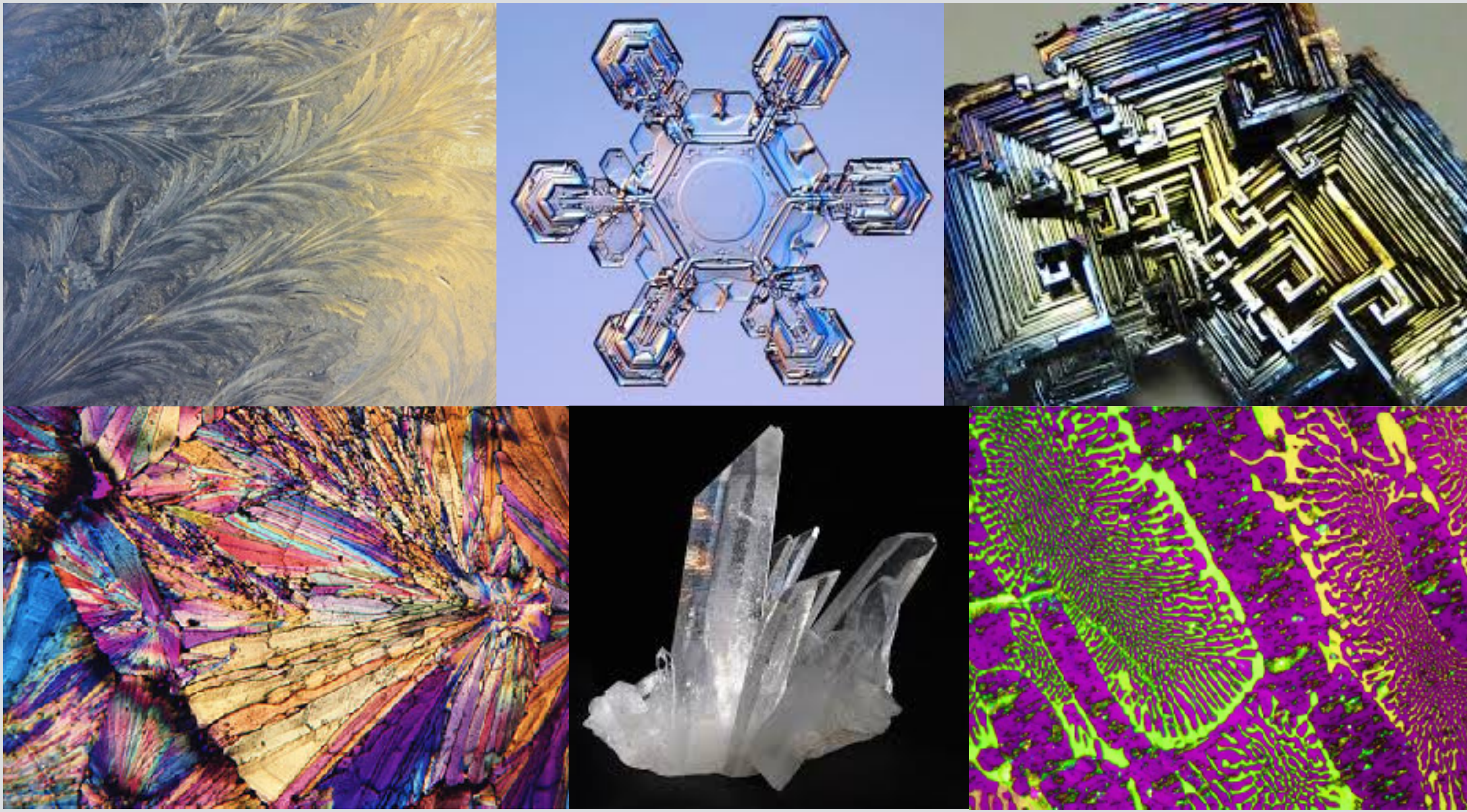
Northeastern University

Yale University

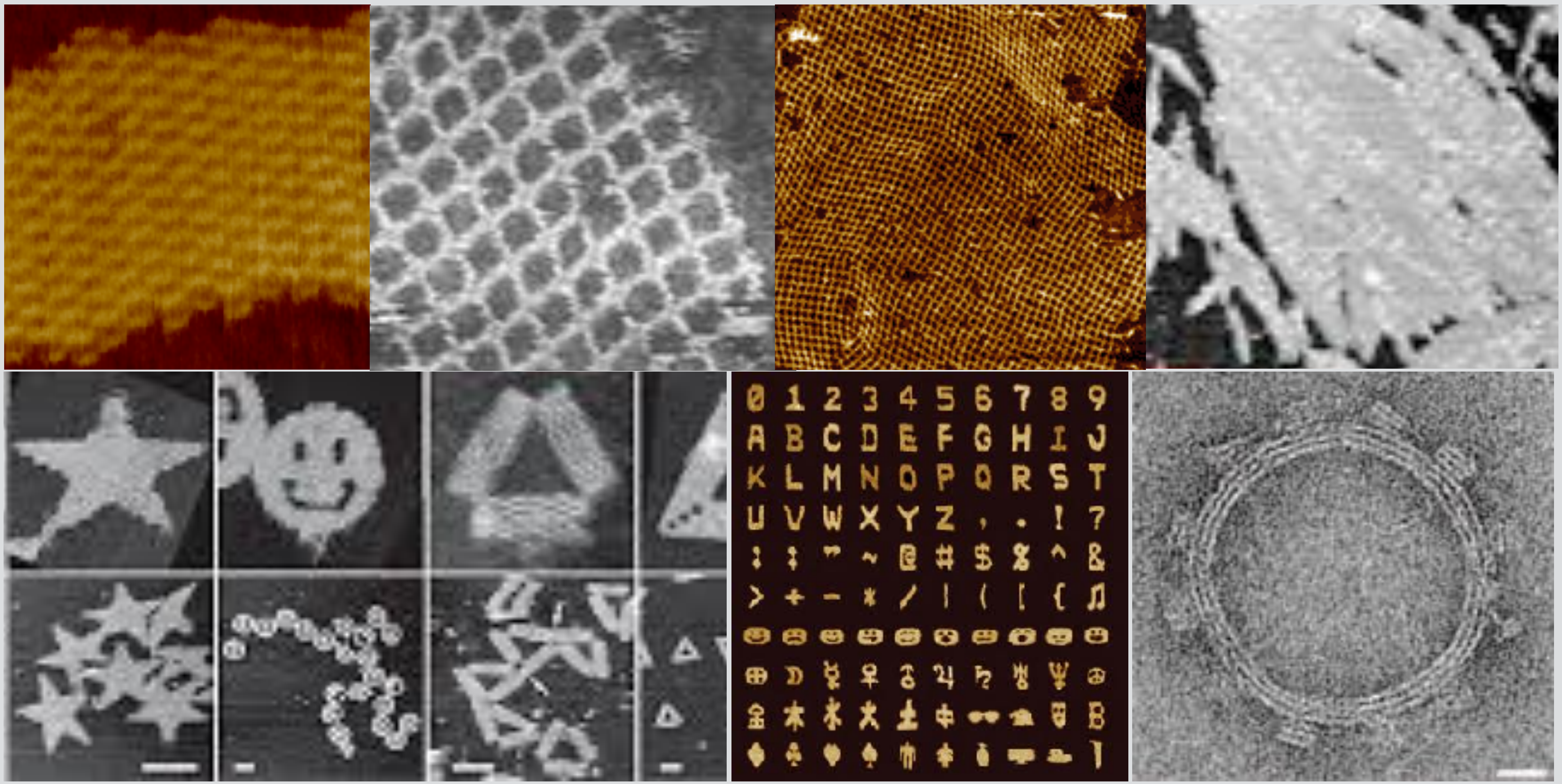
The University of Texas Rio Grande Valley

Self-Assembly

Natural Nanoscale Self-Assembly



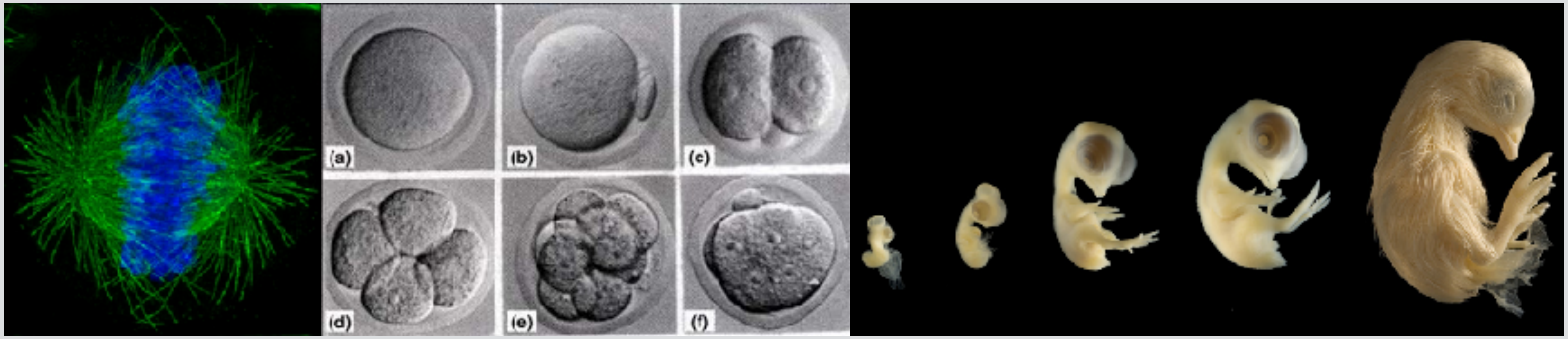
Synthetic Nanoscale Self-Assembly



Passive vs. Active Self-Assembly

- Most current DNA self-assembly uses **passive** growth: static geometry, $n^{O(1)}$ growth rates.

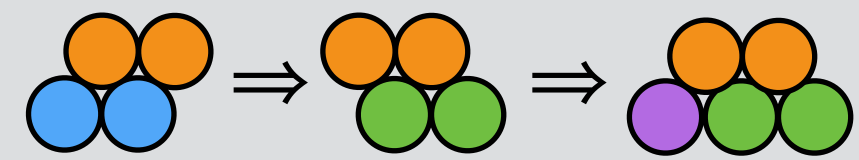
- Some natural systems use **active** growth: dynamic geometry, $2^{O(n)}$ growth rates.



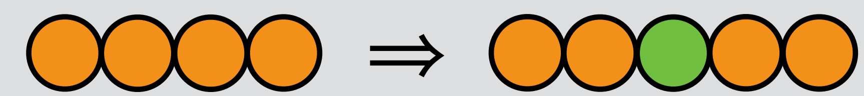
- Here we study an active DNA self-assembly model.

Active Self-Assembly Models

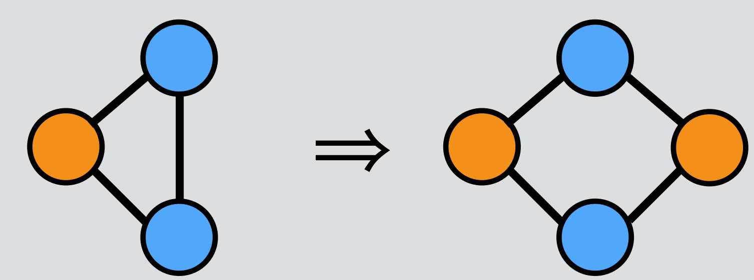
Nubots [Woods et al. ITCS 2012]:
2D, flexible and rigid bonds, stateful particles.



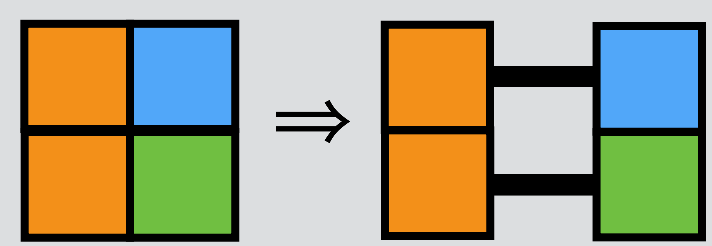
Insertion systems [Dabby, Chen SODA 2013]:
1D, fixed shape, stateless particles.



Graph grammars [Klavins et al. ICRA 2004]:
Geometry-less, stateless particles.



Crystalline robots [Rus, Vona ICRA 1999]:
3D, stateful particles, global communication.



Active Self-Assembly Models

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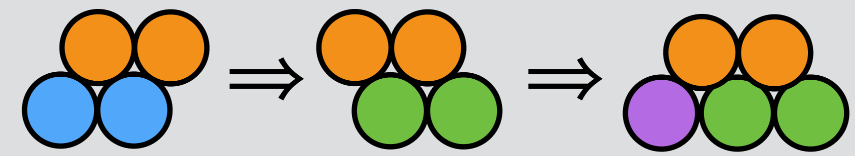

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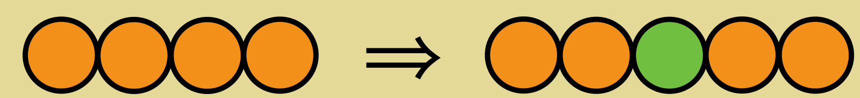

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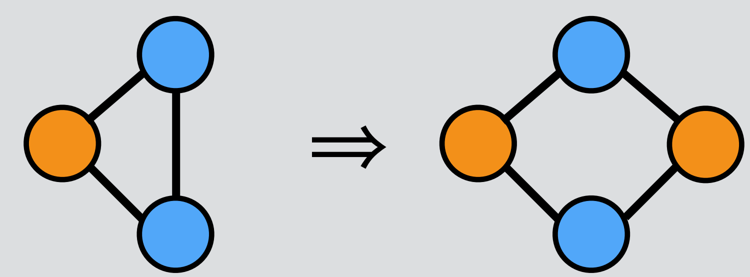

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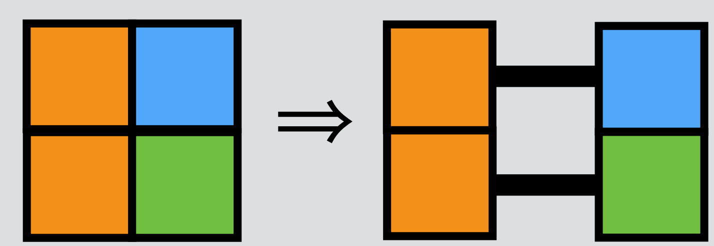
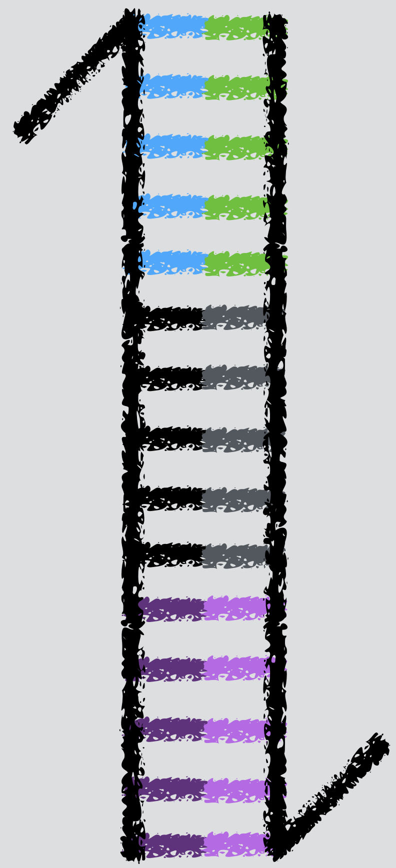
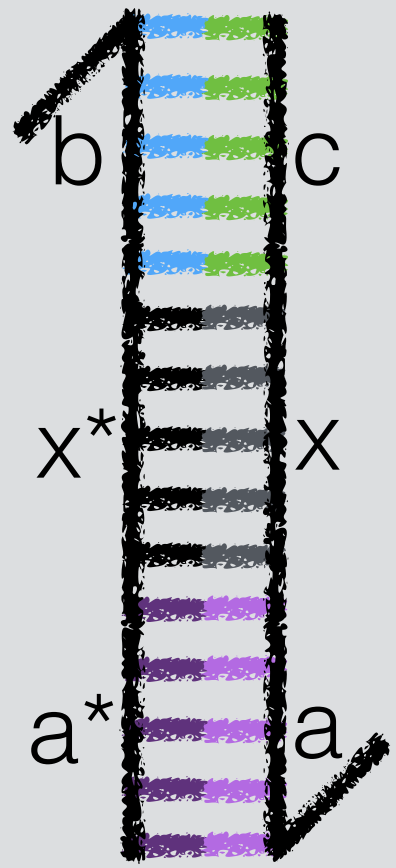


DNA Polymers via Insertion

DNA insertions



DNA insertions



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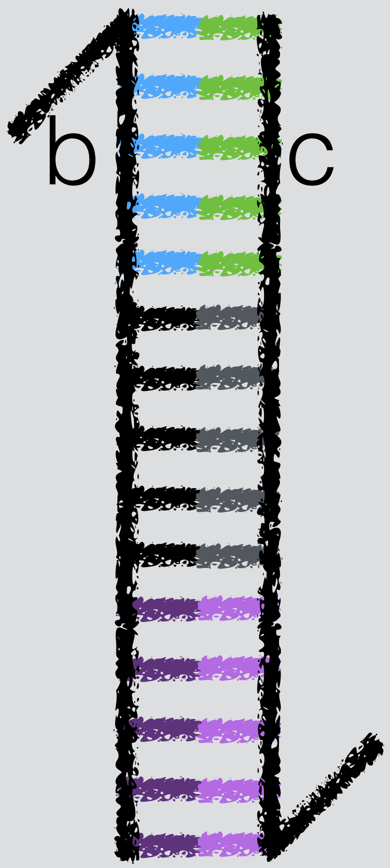

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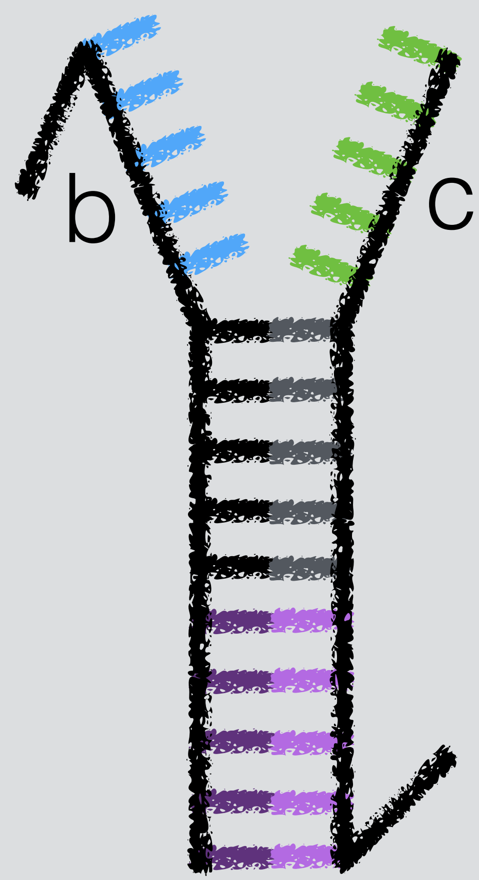

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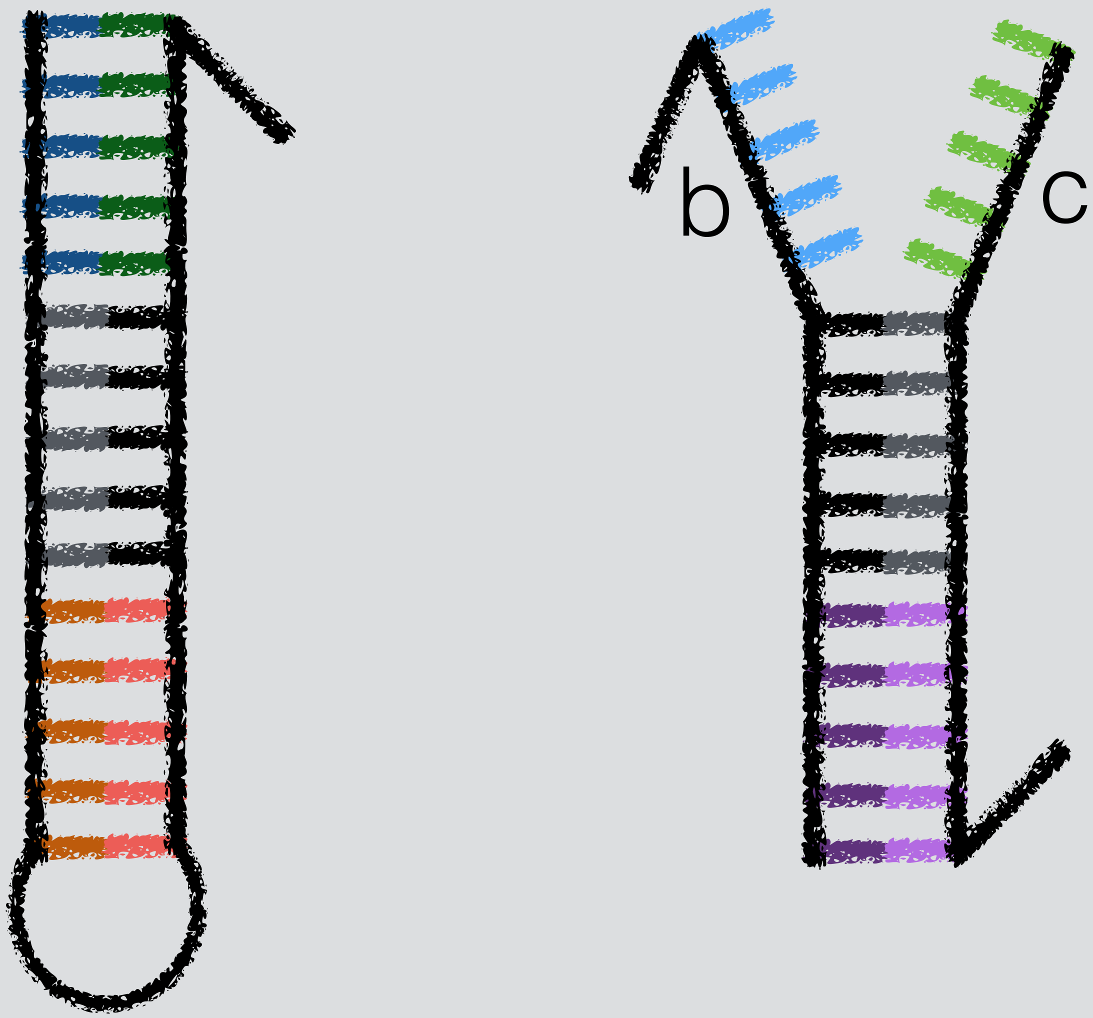

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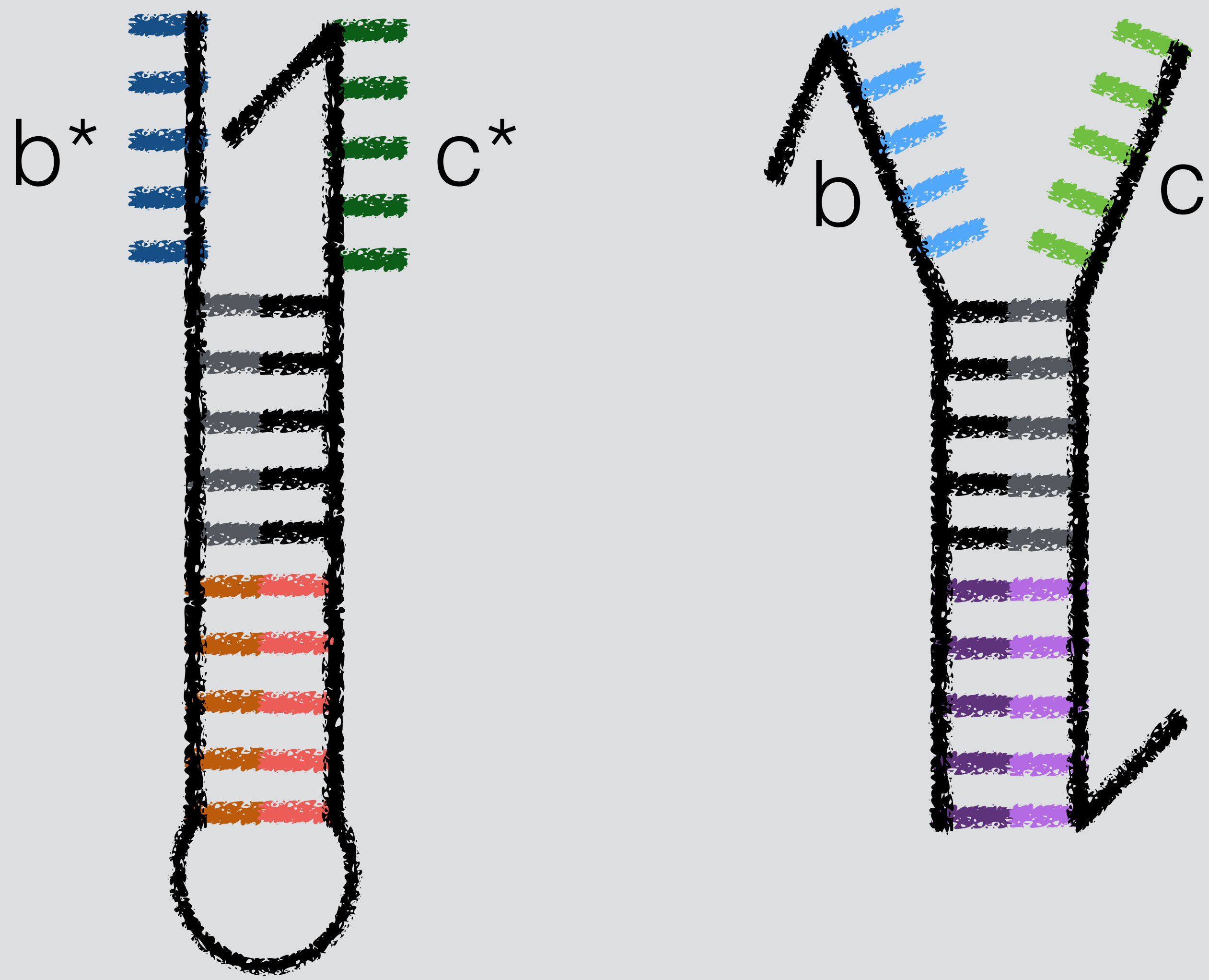

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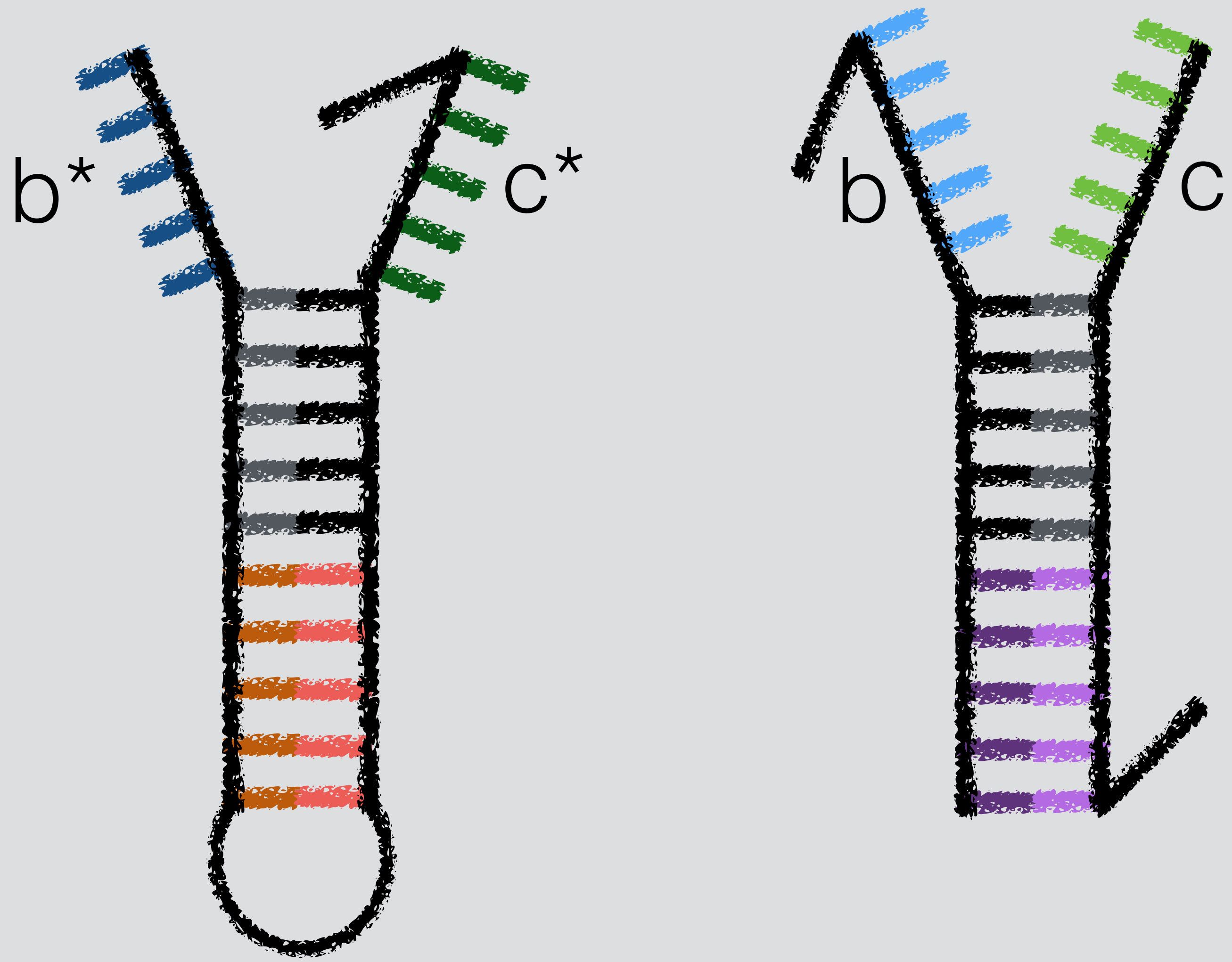

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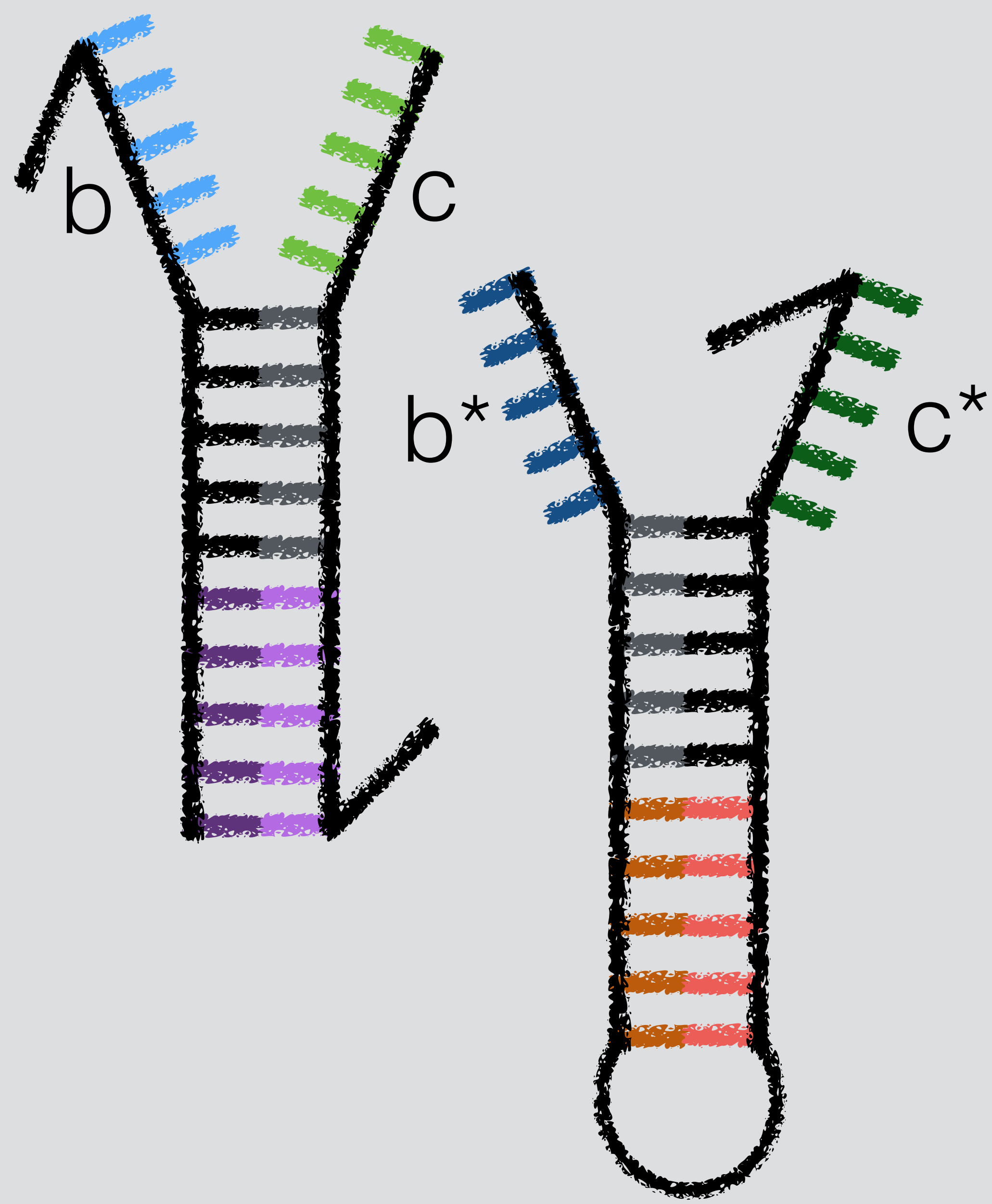

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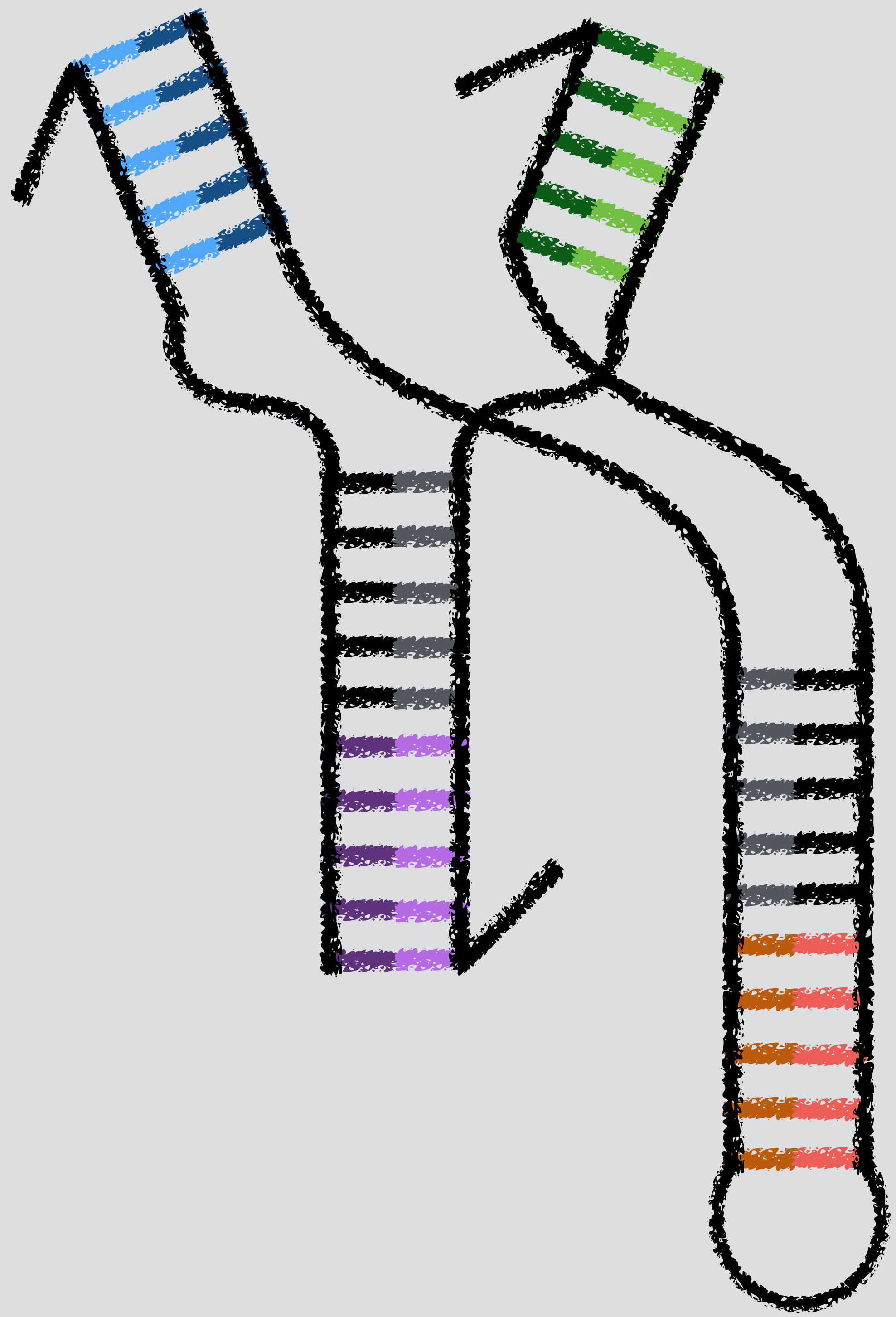

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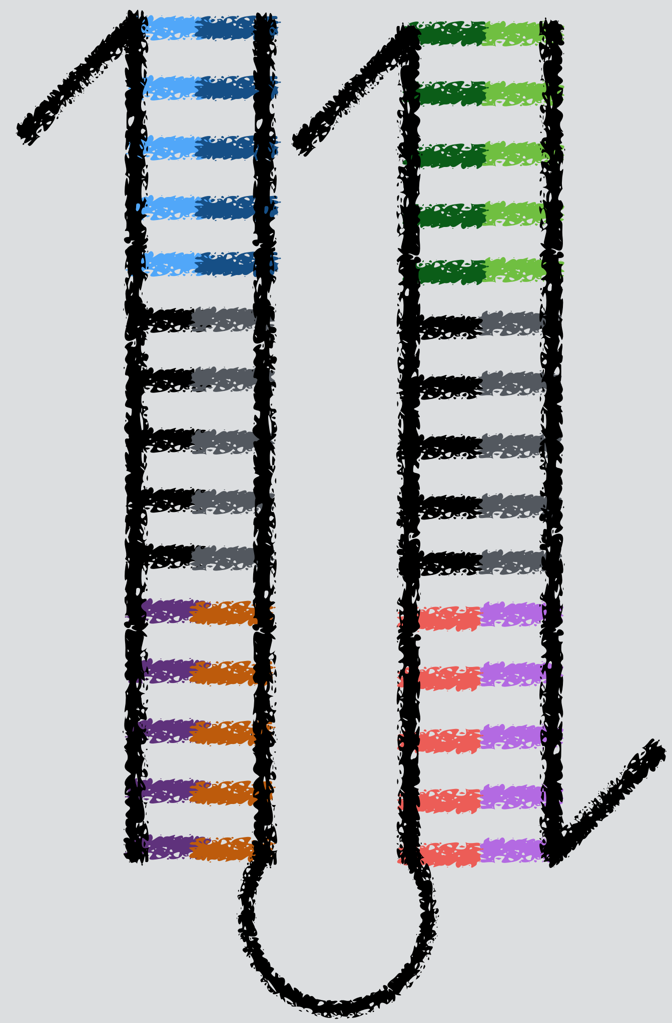
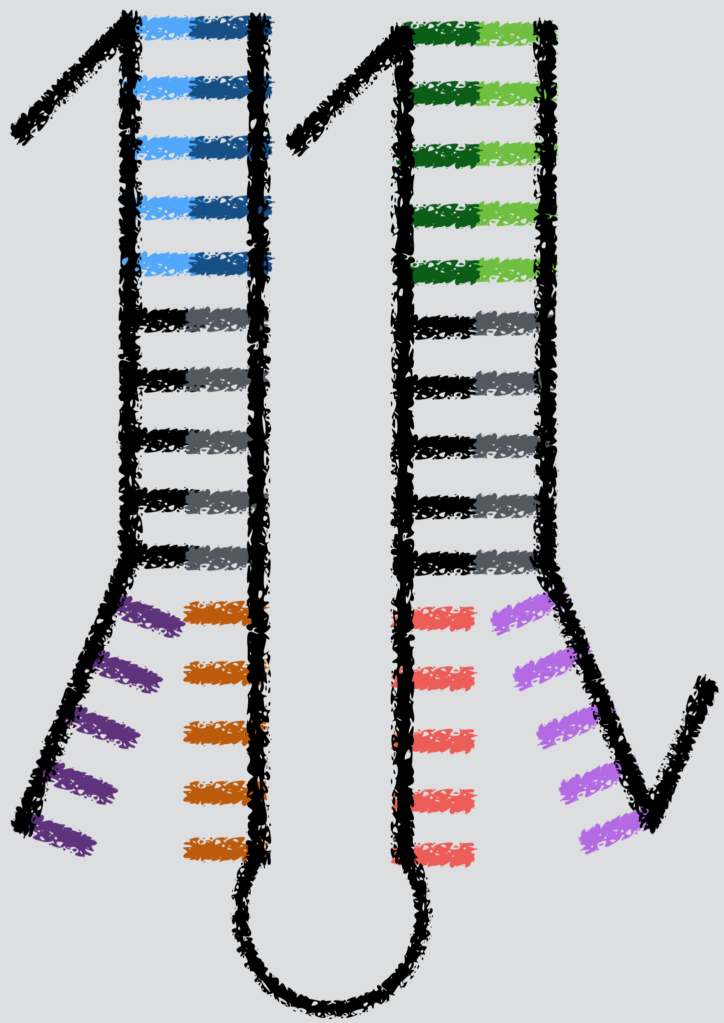


DNA insertions



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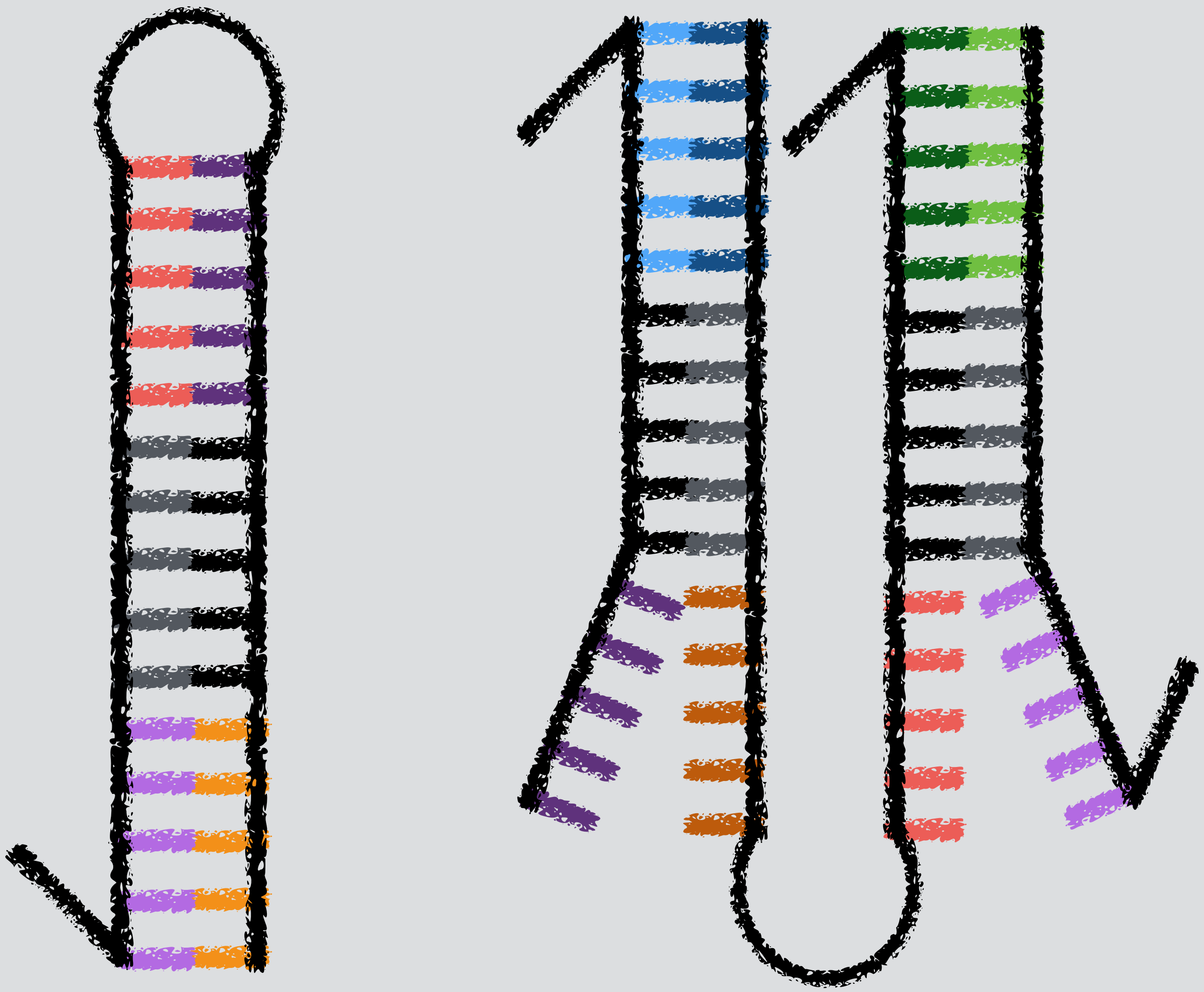
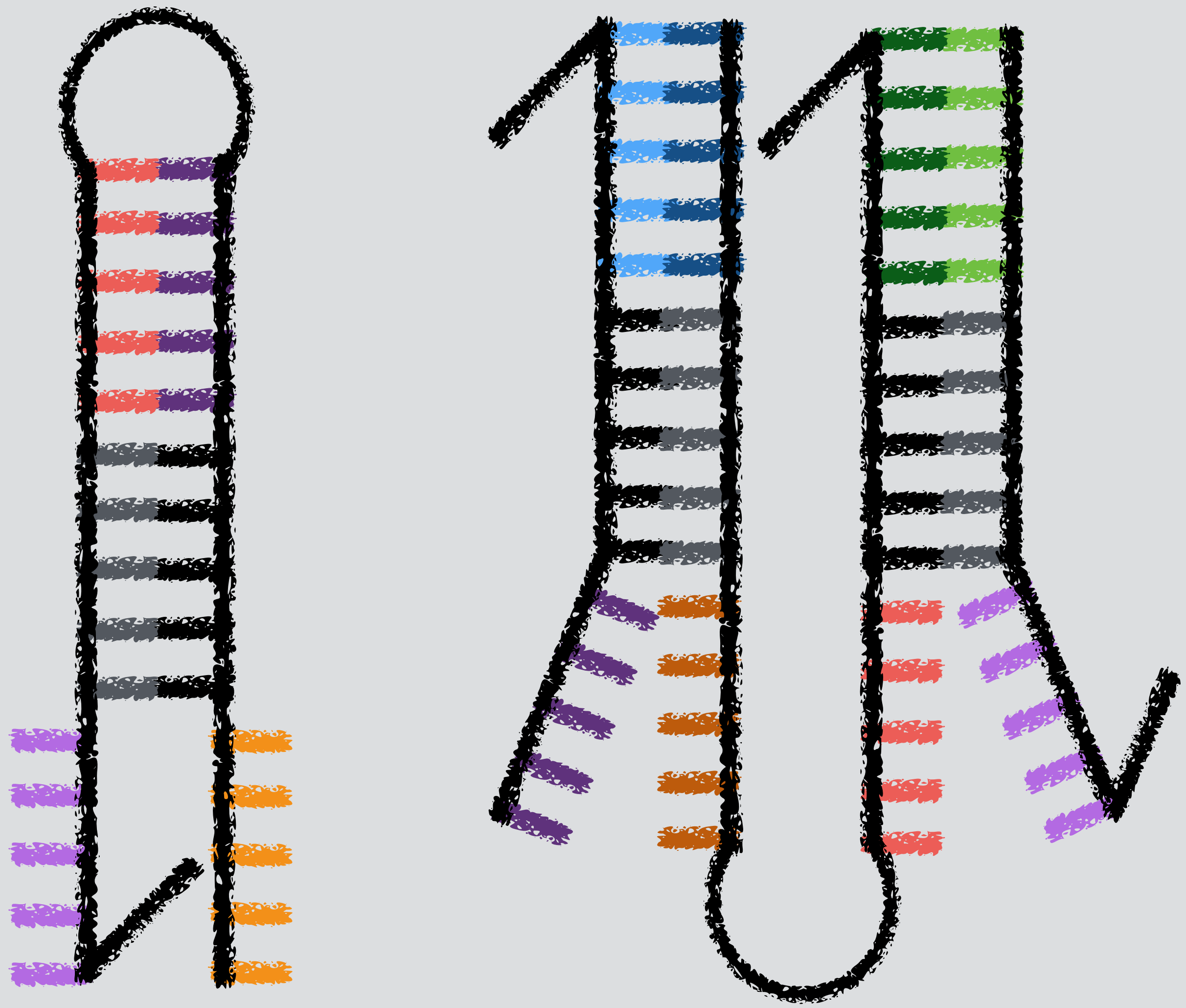
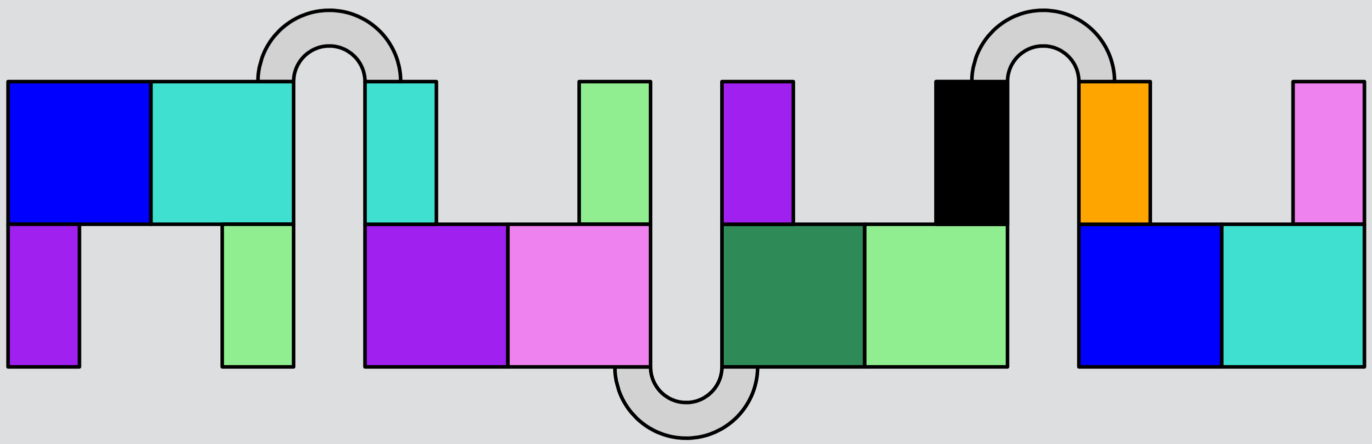


DNA insertions



Insertion systems



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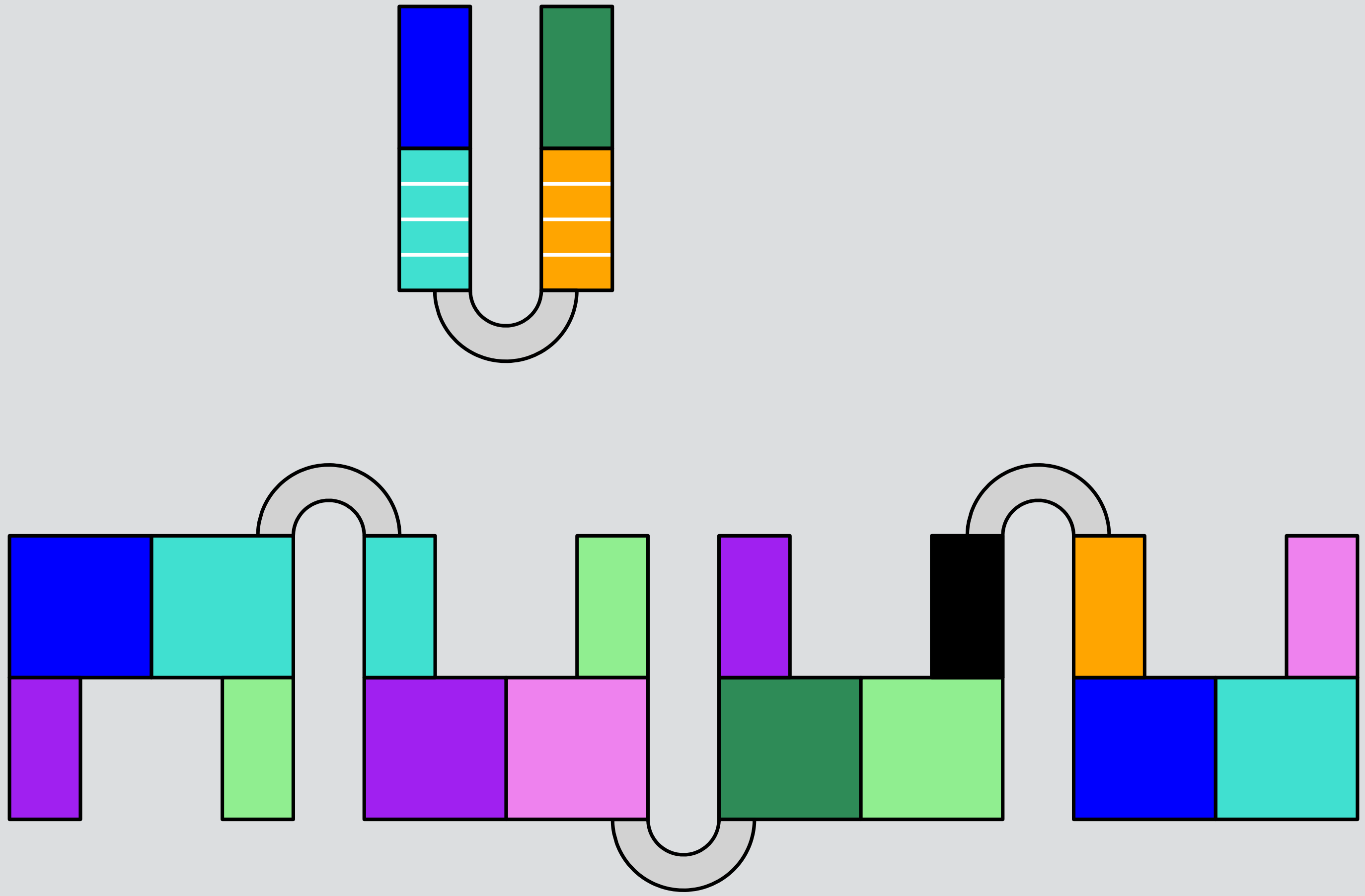
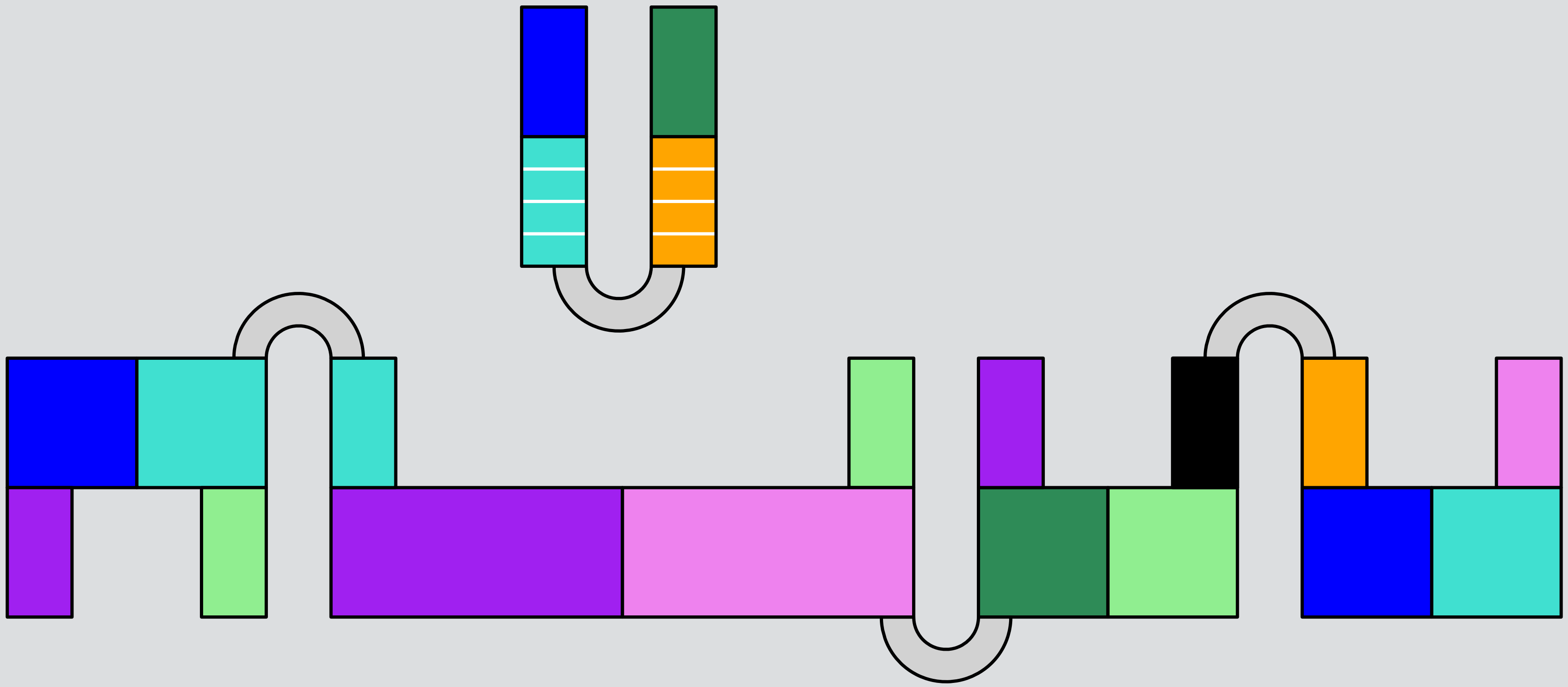
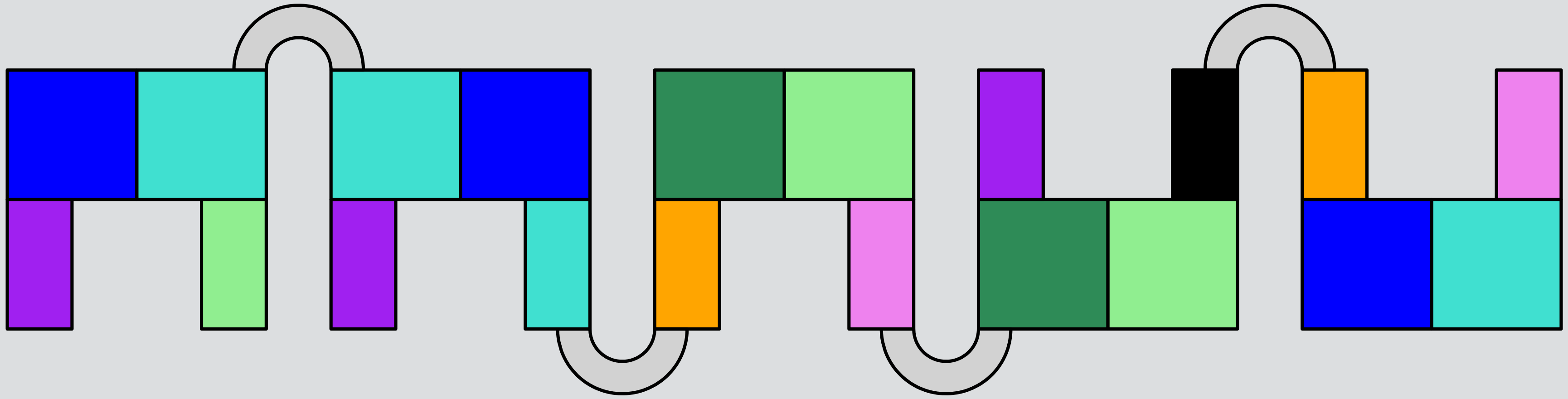


Insertion systems

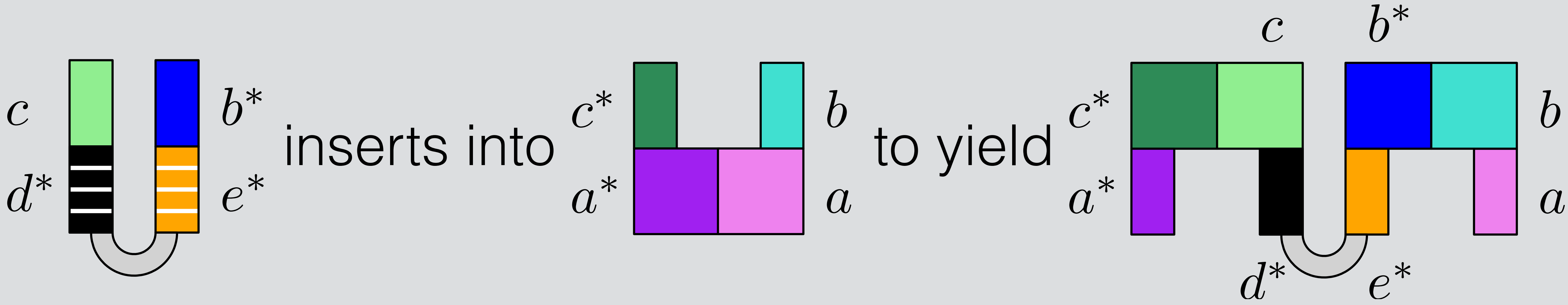


Insertion systems

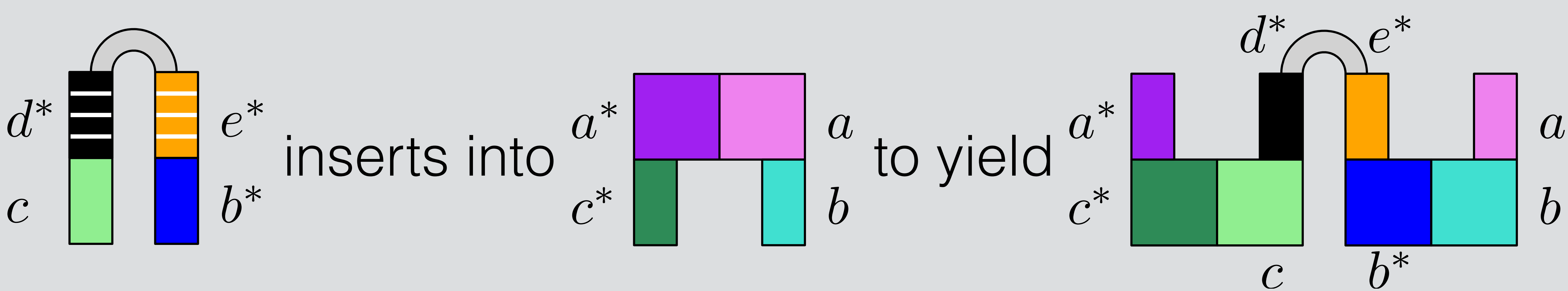


Definitions and Examples

Insertions



$(c, d^*, e^*, b^*)^+$ inserts into $(a^*, c^*)(b, a)$ to yield $(a^*, c^*)(c, d^*, e^*, b^*)(b, a)$



$(d^*, c, b^*, e^*)^-$ inserts into $(c^*, a^*)(a, b)$ to yield $(c^*, a^*)(d^*, c, b^*, e^*)(a, b)$

Insertion system:

Monomer types: $(1,x,2,b)^+$ $(x,2^*,a,3^*)^-$ $(3,x,4,b)^+$

Initiator: $(a,1^*)(b^*,a^*)$

Insertion system:

Monomer types: (1,x,2,b)+ (x,2*,a,3*)- (3,x,4,b)+

Initiator: (a,1*)(b*,a*)

(a,1*)(b*,a*)

Insertion system:

Monomer types: $(1,x,2,b)^{+}$ $(x,2^{*},a,3^{*})^{-}$ $(3,x,4,b)^{+}$

Initiator: $(a,1^{*})(b^{*},a^{*})$

$$(a,1^{*})(b^{*},a^{*})$$
$$\Downarrow$$
$$(a,1^{*})(1,x,2,b)(b^{*},a^{*})$$

Insertion system:

Monomer types: $(1,x,2,b)^+$ $(x,2^*,a,3^*)^-$ $(3,x,4,b)^+$

Initiator: $(a,1^*)(b^*,a^*)$

$$(a,1^*)(b^*,a^*)$$
$$\Downarrow$$
$$(a,1^*)(1,x,2,b)(b^*,a^*)$$
$$\Downarrow$$
$$(a,1^*)(1,x,2,b)(x,2^*,a,3^*)(b^*,a^*)$$

Insertion system:

Monomer types: $(1,x,2,b)^+$ $(x,2^*,a,3^*)^-$ $(3,x,4,b)^+$

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$$(a,1^*)(1,x,2,b)(x,2^*,a,3^*)(3,x,4,b)(b^*,a^*)$$

Terminal polymer of length 5

Insertion Time

- Each monomer type has a concentration in [0,1].
- Concentrations of all types in a system must sum to ≤ 1.
- An insertion occurs after time t where:
    - t is an exponential random variable with rate c.
    - c is the total concentration of insertable monomers.

Insertion system:

Monomer types: $(1,x,2,b)^{+}$ $(x,2^*,a,3^*)^{-}$ $(3,x,4,b)^{+}$

Initiator: (a,1*)(b*,a*)

Insertion system:

Monomer types:	$(1,x,2,b)^{+}$	$(x,2^{*},a,3^{*})^{-}$	$(3,x,4,b)^{+}$
Concentrations:	0.25	0.25	0.5

Initiator: $(a,1^{*})(b^{*},a^{*})$

Insertion system:

Monomer types:	$(1,x,2,b)^+$	$(x,2^*,a,3^*)^-$	$(3,x,4,b)^+$
Concentrations:	0.25	0.25	0.5

Initiator: $(a,1^*)(b^*,a^*)$

$(a,1^*)(b^*,a^*)$

Insertion system:

Monomer types: $(1,x,2,b)^+$ $(x,2^*,a,3^*)^-$ $(3,x,4,b)^+$

Concentrations: 0.25 0.25 0.5

Initiator: $(a,1^*)(b^*,a^*)$

$$(a,1^*)(b^*,a^*)$$
$$\Downarrow t_1$$
$$(a,1^*)(1,x,2,b)(b^*,a^*)$$
$$\Downarrow t_2$$
$$(a,1^*)(1,x,2,b)(x,2^*,a,3^*)(b^*,a^*)$$
$$\Downarrow t_3$$
$$(a,1^*)(1,x,2,b)(x,2^*,a,3^*)(3,x,4,b)(b^*,a^*)$$

Terminal polymer of length 5

Insertion system:

Monomer types: $(1,x,2,b)^{+}$ $(x,2^*,a,3^*)^{-}$ $(3,x,4,b)^{+}$

Concentrations: 0.25 0.25 0.5

Initiator: $(a,1^*)(b^*,a^*)$

$$(a,1^*)(b^*,a^*)$$

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Terminal polymer of length 5

Expected time: $t_1 + t_2 + t_3$, *with*

$E[t_1] = E[t_2] = 4$, $E[t_3] = 2$.

$4 + 4 + 2 = 12$

Insertion system:

Monomer types:	$(1,x,2,b)^+$	$(x,2^*,a,3^*)^-$	$(3,x,4,b)^+$
Concentrations:	0.25	0.25	0.5

Initiator: $(a,1^*)(b^*,a^*)$

$$(a,1^*)(b^*,a^*)$$
$$\Downarrow t_1$$
$$(a,1^*)(1,x,2,b)(b^*,a^*)$$
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$$\Downarrow t_3$$
$$(a,1^*)(1,x,2,b)(x,2^*,a,3^*)(3,x,4,b)(b^*,a^*)$$

Deterministic
(unique terminal polymer)

Terminal polymer of length 5

Expected time: $t_1 + t_2 + t_3$, *with*

$E[t_1] = E[t_2] = 4,\ E[t_3] = 2.$

$4 + 4 + 2 = 12$

Insertion system:

Monomer types: $(1,x,2,b)^+$ $(x,2^*,a,1^*)^-$ $(x,2^*,a,x)^-$

Concentrations:	0.5	0.4	0.1

Initiator: $(a,1^*)(b^*,a^*)$

$$(a,1^*)(b^*,a^*)$$

Insertion system:

Monomer types: $(1,x,2,b)^+$ $(x,2^*,a,1^*)^-$ $(x,2^*,a,x)^-$

Concentrations: 0.5 0.4 0.1

Initiator: $(a,1^*)(b^*,a^*)$

$$(a,1^*)(b^*,a^*)$$
$$\Downarrow t_1$$
$$(a,1^*)(1,x,2,b)(b^*,a^*)$$

Insertion system:

Monomer types: $(1,x,2,b)^+$ $(x,2^*,a,1^*)^-$ $(x,2^*,a,x)^-$

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Insertion system:

Monomer types: $(1,x,2,b)^+$ $(x,2^*,a,1^*)^-$ $(x,2^*,a,x)^-$

Concentrations: 0.5 0.4 0.1

Initiator: $(a,1^*)(b^*,a^*)$

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$$(a,1^*)(1,x,2,b)(b^*,a^*)$$
$$\Downarrow t_2$$
$$(a,1^*)(1,x,2,b)(x,2^*,a,x)(b^*,a^*)$$

Expected time: $t_1 + t_2$, *with*

$E[t_1] = E[t_2] = 2.$

$2 + 2 = 4$

Insertion system:

Monomer types: $(1,x,2,b)^+$ $(x,2^*,a,1^*)^-$ $(x,2^*,a,x)^-$

Concentrations: 0.5 0.4 0.1

Initiator: (a,1*)(b*,a*)

$$(a,1^*)(b^*,a^*)$$
$$\Downarrow t_1$$
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Insertion system:

Monomer types: $(1,x,2,b)^+$ $(x,2^*,a,1^*)^-$ $(x,2^*,a,x)^-$

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$$\Downarrow t_2$$

$$(a,1^*)(1,x,2,b)(x,2^*,a,1^*)(b^*,a^*)$$

Non-deterministic

(≥2 terminal polymers)

Insertion system:

Monomer types: $(1,x,2,b)^+$ $(x,2^*,a,1^*)^-$ $(x,2^*,a,x)^-$

Concentrations:	0.5	0.4	0.1

Initiator: $(a,1^*)(b^*,a^*)$

$$(a,1^*)(b^*,a^*)$$
$$\Downarrow t_1$$
$$(a,1^*)(1,x,2,b)(b^*,a^*)$$
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Insertion system:

Monomer types: $(1,x,2,b)^+$ $(x,2^*,a,1^*)^-$ $(x,2^*,a,x)^-$

Concentrations: 0.5 0.4 0.1

Initiator: $(a,1^*)(b^*,a^*)$

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$$\Downarrow t_3$$
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$$\Downarrow t_4$$
$$(a,1^*)(1,x,2,b)(x,2^*,a,1^*)(1,x,2,b)(x,2^*,a,x)(b^*,a^*)$$

Insertion system:

Monomer types: $(1,x,2,b)^+$ $(x,2^*,a,1^*)^-$ $(x,2^*,a,x)^-$

Concentrations: 0.5 0.4 0.1

Initiator: $(a,1^*)(b^*,a^*)$

$$(a,1^*)(b^*,a^*)$$
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$$\Downarrow t_4$$
$$(a,1^*)(1,x,2,b)(x,2^*,a,1^*)(1,x,2,b)(x,2^*,a,x)(b^*,a^*)$$

Expected time: $t_1 + t_2 + t_3 + t_4$, *with*

$E[t_1] = E[t_2] = E[t_3] = E[t_4] = 2.$

$2 + 2 + 2 + 2 = 8$

Insertion System Goals and Resources

Goal: long polymers of specific lengths constructed quickly using few monomer types.

Resources:

- Monomer type count ≅ program size
- Expected construction time ≅ running time
- Polymer length and specificity ≅ output quality

Prior Results

Expressive Power

<u>Theorem:</u> every insertion system can be expressed as a context-free grammar. [Dabby, Chen 2013]

<u>Theorem:</u> every context-free grammar can be expressed as an insertion system. [HMW 2017]

Polymer Length

Theorem: a system with k monomer types constructing a finite number of polymers can construct:

- polymers of length $2^{\Theta(k^{1/2})}$ [Dabby, Chen 2013]
- polymers of length $2^{\Theta(k^{3/2})}$ [HMW 2017]
- only polymers of length $2^{O(k^{3/2})}$ [HMW 2017]

Construction Time

Theorem: a system constructing a finite number of polymers can **deterministically** construct a polymer of length n in:

- $O(\log^{5/3}(n))$ expected time. [HMW 2017]
- only $\Omega(\log^{5/3}(n))$ expected time. [HMW 2017]

Insertion sequences: repeated insertions into the site resulting from previous insertion.

…u,0)(0,u*…

⇓

…u,0)(0*,1,x,0*)(0,u*…

⇓

…u,0)(x,u*,1*,1*)(0*,1,x,0*)(0,u*…

⇓

…u,0)(x,u*,1*,1*)(1, x, 2, 0)(0*,1,x,0*)(0,u*…

Insertion sequences: repeated insertions into the site resulting from previous insertion.

…u,0)(0,u*…

⇓

…u,0)(0*,1…

⇓

…1*,1*)(0*,1…

⇓

…2, 0)(0*,1…

Insertion sequences: repeated insertions into the site resulting from previous insertion.

…u,0)(0,u*…

⇓

…u,0)(0*,1…

⇓

…1*,1*)(0*,1…

⇓

…2, 0)(0*,1…

Polymer Length

<u>Theorem:</u> a system with k monomer types constructing a finite number of polymers can construct:

- polymers of length $2^{\Theta(k^{1/2})}$ [Dabby, Chen 2013]
- polymers of length $2^{\Theta(k^{3/2})}$ [HMW 2017]
- only polymers of length $2^{O(k^{3/2})}$ [HMW 2017]

Constructing Long Polymers

- Ingredient 1: long insertion sequence with no repeated insertion sites.

$$s_a, s_b)(s_c, s_a^*$$

variables

Use $r+1 = \Theta(k^{1/2})$ values of a, b, c $\Rightarrow \Theta(r^3) = \Theta(k^{3/2})$ insertion sites.

Case:	$b < r$	$b = r,\ c < r$	$b = c = r,\ a < r$
Insertion sequence:	$s_a, s_b)(s_c, s_a^* \overset{O(1)}{\Downarrow} s_a, s_{b+1})(s_c, s_a^*$	$s_a, s_r)(s_c, s_a^* \overset{O(1)}{\Downarrow} s_a, s_0)(s_{c+1}, s_a^*$	$s_a, s_r)(s_r, s_a^* \overset{O(1)}{\Downarrow} s_{a+1}, s_0)(s_0, s_{a+1}^*$
Result:	$++b$	$b = 0,\ ++c$	$b = c = 0,\ ++a$

Triple For-Loop (r = 2)

$$\dots s_0,\ s_0)(s_0,\ s_0{}^{*} \dots$$
$$\Big\Downarrow {\scriptstyle O(1)}$$
$$\dots s_0,\ s_1)(s_0,\ s_0{}^{*} \dots$$
$$\Big\Downarrow {\scriptstyle O(1)}$$
$$\dots s_0,\ s_2)(s_0,\ s_0{}^{*} \dots$$
$$\Big\Downarrow {\scriptstyle O(1)}$$
$$\dots s_0,\ s_0)(s_1,\ s_0{}^{*} \dots$$
$$\Big\Downarrow {\scriptstyle O(1)}$$
$$\dots s_0,\ s_1)(s_1,\ s_0{}^{*} \dots$$
$$\Big\Downarrow {\scriptstyle O(1)}$$
$$\dots s_0,\ s_2)(s_1,\ s_0{}^{*} \dots$$
$$\Big\Downarrow {\scriptstyle O(1)}$$
$$\dots s_0,\ s_0)(s_2,\ s_0{}^{*} \dots$$

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$$\Big\Downarrow {\scriptstyle O(1)}$$
$$\dots s_0,\ s_1)(s_2,\ s_0 \dots$$
$$\Big\Downarrow {\scriptstyle O(1)}$$
$$\dots s_0,\ s_2)(s_2,\ s_0{}^{*} \dots$$
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Case:	$b < r$	$b = r,\ c < r$	$b = c = r,\ a < r$
Insertion sequence:	$s_a, s_b)(s_c, s_a{}^* \Downarrow_{O(1)} s_a, s_{b+1})(s_c, s_a{}^*$	$s_a, s_r)(s_c, s_a{}^* \Downarrow_{O(1)} s_a, s_0)(s_{c+1}, s_a{}^*$	$s_a, s_r)(s_r, s_a{}^* \Downarrow_{O(1)} s_{a+1}, s_0)(s_0, s_{a+1}{}^*$
Result:	++b	b = 0, ++c	b = c = 0, ++a

Constructing Long Polymers

- Ingredient 1: long insertion sequence with no repeated insertion sites.
- Ingredient 2: duplication of each site in sequence.

…3, 4)(7, 3*…

$\Downarrow$ O(1)

…3, 5)(7, 3*… 3, 5)(7, 3*…

$\Downarrow$ O(1)

… 3, 6)(7, 3*… 3, 6)(7, 3*… 3, 6)(7, 3*… 3, 6)(7, 3*…

Constructing Long Polymers

…0,0)(0,0*…

$\Downarrow$ O(1)

…0,0)(1,0*…0,0)(1,0*…

$\Downarrow$ O(1)

…0, 0)(2,0*…0,0)(2,0*…0,0)(2,0*…0,0)(2,0*…

$\Downarrow$ O(1)

⋮

$\Downarrow$ O(1)

…r, r)(r,r*…r, r)(r,r*…r, r)(r,r*…r,r)(r,r*…r,r)(r,r*…r,r)(r,r*…

h

$2^{\Theta(h)}$

Beating $\Omega(\log^{5/3}(n))$ Construction Time

Non-deterministic Construction

$$s_a, s_b)(s_b^*, s_a^*$$

variables

Use $r+1 = \Theta(k^{1/2})$ values of a, b $\Rightarrow \Theta(r^2) = \Theta(k)$ insertion sites.

Case:	$b < r$	$b = r,\ a < r$
Insertion sequence:	$s_a, s_b^*)(s_b^*, s_a^*$ $\Downarrow_{O(1)}$ $s_a, s_{b+1}^*)(s_{b+1}^*, s_a^*$	$s_a, s_r)(s_r^*, s_a^*$ $\Downarrow_{O(1)}$ $s_{a+1}, s_0)(s_0^*, s_{a+1}^*$
Result:	$++b$	$b = 0,\ ++a$

Double For-Loop (r = 2)

$$\ldots s_0,\ s_0)(s_0^*,\ s_0^* \ldots$$
$$\Downarrow_{O(1)}$$
$$\ldots s_0,\ s_1)(s_1^*,\ s_0^* \ldots$$
$$\Downarrow_{O(1)}$$
$$\ldots s_0,\ s_2)(s_2^*,\ s_0^* \ldots$$
$$\Downarrow_{O(1)}$$
$$\ldots s_1,\ s_0)(s_0^*,\ s_1^* \ldots$$
$$\Downarrow_{O(1)}$$
$$\ldots s_1,\ s_1)(s_1^*,\ s_1^* \ldots$$
$$\Downarrow_{O(1)}$$
$$\ldots s_1,\ s_2)(s_2^*,\ s_1^* \ldots$$
$$\Downarrow_{O(1)}$$
$$\ldots s_2,\ s_0)(s_0^*,\ s_2^* \ldots$$

$$\ldots s_2,\ s_0)(s_0^*,\ s_2^* \ldots$$
$$\Downarrow_{O(1)}$$
$$\ldots s_2,\ s_1)(s_1^*,\ s_2 \ldots$$
$$\Downarrow_{O(1)}$$
$$\ldots s_2,\ s_2)(s_2,\ s_2^* \ldots$$

Speedup by non-determinism

$\ldots s_6, s_3)(s_3^*, s_6^* \ldots$

Speedup by non-determinism

$$\ldots s_6, s_3)(s_3^*, s_6^* \ldots$$

$$\Downarrow \text{O(1)} \quad \text{Guess b}$$

$$\ldots s_6, s_3)(s_{f(b+1)}^*, s_6^* \ldots$$

Speedup by non-determinism

$$\ldots s_6, s_3)(s_3^*, s_6^* \ldots$$

$\Downarrow$ O(1) Guess b

$$\ldots s_6, s_3)(s_{f(b+1)}^*, s_6^* \ldots$$

$\Downarrow$ O(1) If guessed b = 3, guess a

$$\ldots s_{f(a)}, s_{f(b+1)})(s_{f(b+1)}^*, s_6^* \ldots$$

Speedup by non-determinism

$$\ldots s_6, s_3)(s_3^*, s_6^* \ldots$$

$\Downarrow$ O(1) Guess b

$$\ldots s_6, s_3)(s_{f(b+1)}^*, s_6^* \ldots$$

$\Downarrow$ O(1) If guessed b = 3, guess a

$$\ldots s_{f(a)}, s_{f(b+1)})(s_{f(b+1)}^*, s_6^* \ldots$$

$\Downarrow$ O(1) If guessed a = 6

$$\ldots s_{f(a)}, s_{f(b+1)})(s_{f(b+1)}^*, s_{f(a)}^* \ldots$$

Speedup by non-determinism

$$\ldots s_6, s_3)(s_3{}^*, s_6{}^* \ldots$$

$\Downarrow$ O(1) Guess b

$$\ldots s_6, s_3)(s_{f(b+1)}{}^*, s_6{}^* \ldots$$

$\Downarrow$ O(1) If guessed b = 3, guess a

$$\ldots s_{f(a)}, s_{f(b+1)})(s_{f(b+1)}{}^*, s_6{}^* \ldots$$

$\Downarrow$ O(1) If guessed a = 6

$$\ldots s_{f(6)}, s_{f(4)})(s_{f(4)}{}^*, s_{f(6)}{}^* \ldots$$

Speedup by non-determinism

$$\ldots s_6, s_3)(s_3^*, s_6^* \ldots$$

$\Downarrow$ O(1) Guess b

$$\ldots s_6, s_3)(s_{f(b+1)}^*, s_6^* \ldots$$

$\Downarrow$ O(1) If guessed b = 3, guess a

$$\ldots s_{f(a)}, s_{f(b+1)})(s_{f(b+1)}^*, s_6^* \ldots$$

$\Downarrow$ O(1) If guessed a = 6

$$\ldots s_{f(6)}, s_{f(4)})(s_{f(4)}^*, s_{f(6)}^* \ldots$$

$\Downarrow$ O(1)

$$\ldots s_6, s_4)(s_4^*, s_6^* \ldots$$

Speedup by non-determinism

$\ldots s_6, s_3)(s_3^*, s_6^* \ldots$

Speedup by non-determinism

$$\ldots s_6, s_3)(s_3^*, s_6^* \ldots$$

$$\Big\Downarrow^{O(1)} \text{ Guess b}$$

$$\ldots s_6, s_3)(s_{f(b+1)}^*, s_6^* \ldots$$

Speedup by non-determinism

$$\ldots s_6, s_3)(s_3^*, s_6^* \ldots$$

O(1) $\Downarrow$ Guess b

$$\ldots s_6, s_3)(s_{f(b+1)}^*, s_6^* \ldots$$

O(1) $\Downarrow$ If guessed b $\neq$ 3, halt

$$\times$$

Speedup by non-determinism

$\ldots s_6, s_3)(s_3^*, s_6^* \ldots$

Speedup by non-determinism

$$\ldots s_6, s_3)(s_3^*, s_6^* \ldots$$

$$\Downarrow^{O(1)} \text{ Guess b}$$

$$\ldots s_6, s_3)(s_{f(b+1)}^*, s_6^* \ldots$$

Speedup by non-determinism

$$\ldots s_6, s_3)(s_3^*, s_6^* \ldots$$

$$\overset{O(1)}{\Downarrow} \text{ Guess } b$$

$$\ldots s_6, s_3)(s_{f(b+1)}^*, s_6^* \ldots$$

$$\overset{O(1)}{\Downarrow} \text{ If guessed } b = 3\text{, guess } a$$

$$\ldots s_{f(a)}, s_{f(b+1)})(s_{f(b+1)}^*, s_6^* \ldots$$

Speedup by non-determinism

$$\ldots s_6, s_3)(s_3{}^*, s_6{}^* \ldots$$

$O(1)$ $\Downarrow$ Guess b

$$\ldots s_6, s_3)(s_{f(b+1)}{}^*, s_6{}^* \ldots$$

$O(1)$ $\Downarrow$ If guessed b = 3, guess a

$$\ldots s_{f(a)}, s_{f(b+1)})(s_{f(b+1)}{}^*, s_6{}^* \ldots$$

$O(1)$ $\Downarrow$ If guessed a ≠ 6, halt

$$\times$$

Why does guessing give a speed-up?

Deterministic Construction

$$\ldots s_6, s_3)(s_5, s_6^* \ldots$$

$$\Downarrow_{O(1)}$$

$$\ldots s_6, s_4)(s_5^*, s_6^* \ldots$$

Incrementing uses *unique* monomers.

Unique monomers insertions are slow.

Speedup by non-determinism

$$\ldots S_6, S_3)(S_3{}^*, S_6{}^* \ldots$$

$$\overset{O(1)}{\Downarrow} \quad \text{Guess b}$$

$$\ldots S_6, S_3)(S_{f(b+1)}{}^*, S_6{}^* \ldots$$

$$\overset{O(1)}{\Downarrow} \quad \text{If guessed b = 3, guess a}$$

$$\ldots S_{f(a)}, S_{f(b+1)})(S_{f(b+1)}{}^*, S_6{}^* \ldots$$

$$\overset{O(1)}{\Downarrow} \quad \text{If guessed a = 6}$$

$$\ldots S_{f(a)}, S_{f(b+1)})(S_{f(b+1)}{}^*, S_{f(a)}{}^* \ldots$$

Speedup by non-determinism

$$s_6,s_3)(s_3{}^*,s_6{}^*$$

$$\Downarrow_{O(1)} \text{ Guess b}$$

$$s_6,s_3)(s_{f(b+1)}{}^*,s_6{}^*$$

$$s_6,s_5)(s_5{}^*,s_6{}^*$$

$$\Downarrow_{O(1)} \text{ Guess b}$$

$$s_6,s_5)(s_{f(b+1)}{}^*,s_6{}^*$$

$$s_6,s_8)(s_8{}^*,s_6{}^*$$

$$\Downarrow_{O(1)} \text{ Guess b}$$

$$s_6,s_8)(s_{f(b+1)}{}^*,s_6{}^*$$

$$s_6,s_{11})(s_{11}{}^*,s_6{}^*$$

$$\Downarrow_{O(1)} \text{ Guess b}$$

$$s_6,s_{11})(s_{f(b+1)}{}^*,s_6{}^*$$

Speedup by non-determinism

$S_6,S_3)(S_3{}^*,S_6{}^*$ $S_6,S_5)(S_5{}^*,S_6{}^*$

$\Downarrow$ Guess b $\Downarrow$ Guess b

$S_6,S_3)(S_{f(b+1)}{}^*,S_6{}^*$ $S_6,S_5)(S_{f(b+1)}{}^*,S_6{}^*$

The same set of monomers are insertable to *all* of these sites.

$S_6,S_8)(S_8{}^*,S_6{}^*$ $S_6,S_{11})(S_{11}{}^*,S_6{}^*$

$\Downarrow$ Guess b $\Downarrow$ Guess b

$S_6,S_8)(S_{f(b+1)}{}^*,S_6{}^*$ $S_6,S_{11})(S_{f(b+1)}{}^*,S_6{}^*$

Speedup by non-determinism

- Sites $s_a, s_b)(s_b^*, s_a^*$ with $r = \Theta(k^{1/2})$ values for a, b
  - So $k = \Theta(\log(n))$
- Every site accepts $\Theta(k^{1/2})$ monomers:
  $\Omega(1/k^{1/2})$ total concentration.
- Expected insertion time is $O(k^{1/2}) = O(\log^{1/2}(n))$.
- Total expected construction time is $O(\log^{3/2}(n))$. beating $\Omega(\log^{5/3}(n))$
- Caveat: halted insertion sequences ⇒ shorter polymers.

Lower Bound for Non-Deterministic Construction Time

Polymer construction

Theorem: a system constructing a finite number of polymers can **deterministically** construct a polymer of length n in:

- $O(\log^{5/3}(n))$ expected time using $\Theta(\log^{2/3}(n))$ types.
- only $\Omega(\log^{5/3}(n))$ expected time.

Theorem: a system constructing a finite number of polymers can **non-deterministically** construct a polymer of length n in:

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Types vs Speed Tradeoff

Is it possible to construct a polymer using $O(\log^{2/3}(n))$ monomer types in $O(\log^{3/2}(n))$ expected time?

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Theorem: in a system constructing a finite number of polymers, constructing a polymer of length n using k monomer types takes $\Omega(\log^2(n)/k^{1/2})$ expected time.

Types vs Speed Tradeoff

Is it possible to construct a polymer using $O(\log^{2/3}(n))$ monomer types in $O(\log^{3/2}(n))$ expected time? No

Theorem: in a system constructing a finite number of polymers, constructing a polymer of length n using k monomer types takes $\Omega(\log^2(n)/k^{1/2})$ expected time.

$O(\log^{2/3}(n))$ types ⇒ $\Omega(\log^{5/3}(n))$ expected time.

$O(\log^{3/2}(n))$ expected time ⇒ $\Omega(\log(n))$ types.

Open Problems

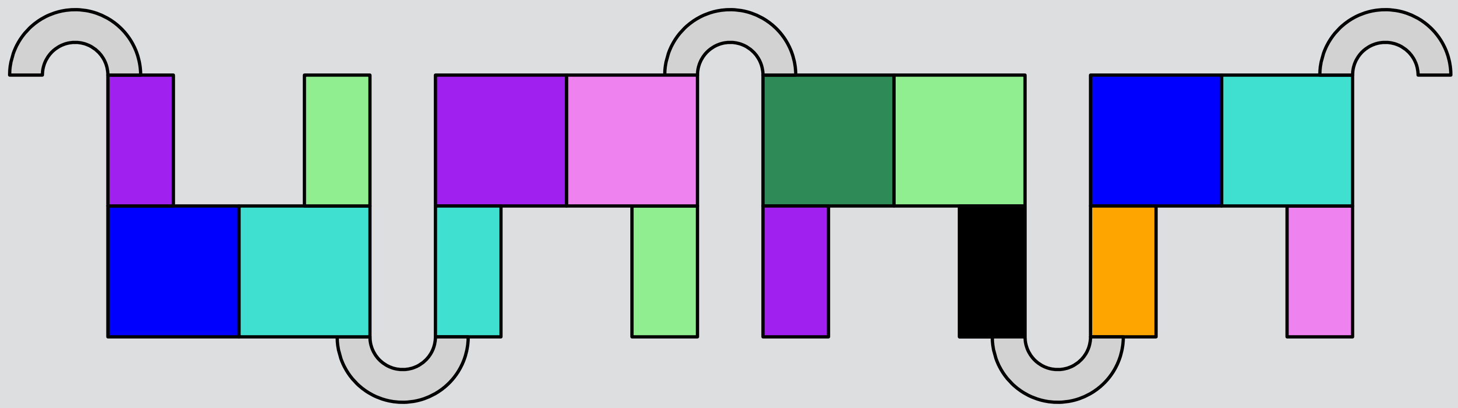
Trade-off systems matching lower bound?

- Known: $O(\log^{5/3}(n))$ expected time using $\Theta(\log^{2/3}(n))$ types.
- Known: $O(\log^{3/2}(n))$ expected time using $\Theta(\log(n))$ types.
- $O(\log^2(n)/k^{1/2})$ expected time using $\log^{2/3}(n) \leq k \leq \log(n)$ types.

Reduce shorter "junk" assemblies (currently $2^{\Theta(n\log\log(n))}$)

- Practical goal: targeted polymer length.
- $O(1)$ "junk" assemblies possible?

Non-Determinism Reduces Construction Time in Active Self-Assembly Using an Insertion Primitive



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