Rate-Independent Constructs for Chemical Computation

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Appendix: Raise-to-a-Power Reactions

We present chemical reactions that implement the pseudo-code presented in the text.

System Initialization We assume that an external source injects some quantity of *begin* at the outset. This type is immediately is split into two types, g^1 and g^7, which will be used to copy x to y (for the line of code `y = x`) and to decrement p (for the line of code `p = p - 1`), respectively. This initializations takes care of the steps before the first `while` statement.

$$begin \xrightarrow{\text{fast}} g^1 + g^7 \tag{1}$$

Copy x to y $\left[g^1\right]$

$$x + g^1 \xrightarrow{\text{slow}} xy + g^1 \tag{2}$$
$$g^1 + x_{\text{ab}} \xrightarrow{\text{slow}} \varnothing \tag{3}$$
$$xy + g^1_{\text{ab}} \xrightarrow{\text{slow}} x + y \tag{4}$$

Loop Restart Our condition for restarting the main loop is that we still have p present in the system, and that we are not currently somewhere in the middle of the loop. The chemical type *done* is produced at the end of each loop from reactions 63 through 75 below. We also will wait until our post-loop cleanup in reactions 76 through 78 below is complete. At the start of each loop, we produce an injection of g^2 and g^7; these initiate the loop.

$$st_{\text{ab}} + cyc_{\text{ab}} + g^6_{\text{ab}} + stgo_{\text{ab}} + done + p \xrightarrow{\text{slow}} go^{\text{P}} + done + p \tag{5}$$
$$go^{\text{P}} + st \xrightarrow{\text{fast}} st \tag{6}$$
$$go^{\text{P}} + cyc \xrightarrow{\text{fast}} cyc \tag{7}$$
$$go^{\text{P}} + g^6 \xrightarrow{\text{fast}} g_6 \tag{8}$$
$$go^{\text{P}} + stgo \xrightarrow{\text{fast}} stgo \tag{9}$$
$$go^{\text{P}} \xrightarrow{\text{slow}} go + stgo \tag{10}$$
$$go \xrightarrow{\text{fast}} g^2 + g^7 \tag{11}$$
$$w + done \xrightarrow{\text{fast}} w \tag{12}$$
$$xw + done \xrightarrow{\text{fast}} xw \tag{13}$$
$$cyc + stgo \xrightarrow{\text{slow}} cyc \tag{14}$$

Copy x to w (once each loop) $\left[g^2\right]$ First, we take care of `w = x`.

$$x + g^2 \xrightarrow{\text{slow}} xw + g^2 \tag{15}$$
$$x_{\text{ab}} + g^2 \xrightarrow{\text{slow}} \varnothing \tag{16}$$
$$g^2_{\text{ab}} + xw \xrightarrow{\text{slow}} x + w \tag{17}$$

Loop-Running Indicator We produce a chemical type *cyc* whenever we are executing a loop. This is to ensure that our modules will not inadvertently fire when we do not wish them to do so.

$$w \xrightarrow{\text{slow}} w + cyc \tag{18}$$
$$2\,cyc \xrightarrow{\text{fast}} cyc \tag{19}$$

Multiply Loop Start The inner `while` loop is our multiply operation, handled by the next three groups of reactions.

$$w + w'_{\text{ab}} + yd_{\text{ab}} \xrightarrow{\text{slow}} w + g^{34\text{P}} \tag{20}$$
$$g^{34\text{P}} + w' \xrightarrow{\text{fast}} w' \tag{21}$$
$$g^{34\text{P}} + yd \xrightarrow{\text{fast}} yd \tag{22}$$
$$g^{34\text{P}} \xrightarrow{\text{slow}} g^3 + g^4 \tag{23}$$

Copy y to d (multiply loop) $\left[g^3\right]$

$$y + g^3 \xrightarrow{\text{fast}} yd + g^3 \tag{24}$$
$$g^3 + y_{\text{ab}} \xrightarrow{\text{slow}} \varnothing \tag{25}$$
$$g^3_{\text{ab}} + yd \xrightarrow{\text{slow}} y + d \tag{26}$$

Decrement w $\left[g^4\right]$

$$w + g^4 \xrightarrow{\text{fast}} w' + g^4 \tag{27}$$
$$g^4 + w_{\text{ab}} \xrightarrow{\text{slow}} \varnothing \tag{28}$$
$$g^4_{\text{ab}} \xrightarrow{\text{slow}} g'^4_{\text{ab}} \tag{29}$$
$$2\,w' + g'^4_{\text{ab}} \xrightarrow{\text{fast}} w' + w + w^{\text{rx}} \tag{30}$$
$$w^{\text{rx}} \xrightarrow{\text{slow}} \varnothing \tag{31}$$
$$w' + w^{\text{rx}}_{\text{ab}} + g'^4_{\text{ab}} \xrightarrow{\text{slow}} \varnothing \tag{32}$$
$$2\,g'^4_{\text{ab}} \xrightarrow{\text{slow}} g'^4_{\text{ab}} \tag{33}$$
$$g'^4_{\text{ab}} + g^4 \xrightarrow{\text{fast}} g^4 \tag{34}$$

End of Multiply Detection Once the multiplication operation has completed, we produce g^5, enabling the next step:

$$\begin{aligned}
w_{\mathrm{ab}} + w'_{\mathrm{ab}} + g^2_{\mathrm{ab}} & & \\
+xw_{\mathrm{ab}} + st_{\mathrm{ab}} + done_{\mathrm{ab}} & \xrightarrow{\text{slow}} & g^{5\mathrm{P}} && (35)\\
g^{5\mathrm{P}} + w & \xrightarrow{\text{fast}} & w && (36)\\
g^{5\mathrm{P}} + w' & \xrightarrow{\text{fast}} & w' && (37)\\
g^{5\mathrm{P}} + g^2 & \xrightarrow{\text{fast}} & g^2 && (38)\\
g^{5\mathrm{P}} + xw & \xrightarrow{\text{fast}} & xw && (39)\\
g^{5\mathrm{P}} + st & \xrightarrow{\text{fast}} & st && (40)\\
g^{5\mathrm{P}} + done & \xrightarrow{\text{fast}} & done && (41)\\
g^{5\mathrm{P}} + cyc & \xrightarrow{\text{slow}} & g^5 + cyc && (42)
\end{aligned}$$

Clear y $\left[g^5\right]$ We must take care of the lines `y = d` and `d = 0`. First, we clear our previous quantity of y.

$$\begin{aligned}
g^5 + y & \xrightarrow{\text{slow}} & g^5 && (43)\\
y_{\mathrm{ab}} + g^5 & \xrightarrow{\text{slow}} & \varnothing && (44)
\end{aligned}$$

Inhibit production of g^5 We stop production of g^5 so that we may preserve the quantity of y that we are going to receive from d.

$$\begin{aligned}
y_{\mathrm{ab}} + yd_{\mathrm{ab}} & \xrightarrow{\text{slow}} & st^{\mathrm{P}} && (45)\\
st^{\mathrm{P}} + y & \xrightarrow{\text{fast}} & y && (46)\\
st^{\mathrm{P}} + yd & \xrightarrow{\text{fast}} & yd && (47)\\
st^{\mathrm{P}} + g^5 & \xrightarrow{\text{slow}} & st + g^5 && (48)
\end{aligned}$$

Set y **to** d $\left[g^6\right]$ Finally, we transfer d to y, clearing d in the process.

$$\begin{aligned}
y_{\mathrm{ab}} + g^5_{\mathrm{ab}} + yd_{\mathrm{ab}} & \xrightarrow{\text{slow}} & g^{6\mathrm{P}} && (49)\\
g^{6\mathrm{P}} + y & \xrightarrow{\text{fast}} & y && (50)\\
g^{6\mathrm{P}} + g^5 & \xrightarrow{\text{fast}} & g^5 && (51)\\
g^{6\mathrm{P}} + yd & \xrightarrow{\text{fast}} & yd && (52)\\
g^{6\mathrm{P}} + d + st & \xrightarrow{\text{slow}} & g^6 + d + st && (53)\\
g^6 + d & \xrightarrow{\text{slow}} & g^6 + y && (54)
\end{aligned}$$

Decrement p $\left[g^7\right]$ The decrement of p is used several in two distinct cases, but we only need one instance of the module for our system.

$$p + g^7 \xrightarrow{\text{fast}} p' + g^7 \tag{55}$$
$$g^7 + p_{\text{ab}} \xrightarrow{\text{slow}} \varnothing \tag{56}$$
$$g^7_{\text{ab}} \xrightarrow{\text{slow}} g'^7_{\text{ab}} \tag{57}$$
$$2\,p' + g'^7_{\text{ab}} \xrightarrow{\text{fast}} p' + p + p^{\text{rx}} \tag{58}$$
$$p^{\text{rx}} \xrightarrow{\text{slow}} \varnothing \tag{59}$$
$$p' + p^{\text{rx}}_{\text{ab}} + g'^7_{\text{ab}} \xrightarrow{\text{slow}} \varnothing \tag{60}$$
$$2\,g'^7_{\text{ab}} \xrightarrow{\text{slow}} g'^7_{\text{ab}} \tag{61}$$
$$g'^7_{\text{ab}} + g^7 \xrightarrow{\text{fast}} g^7 \tag{62}$$

End-of-Loop Detection We know that we have finished a loop when all operations within and prior to the loop have completed.

$$\begin{aligned} &yd_{\text{ab}} + d_{\text{ab}} + go_{\text{ab}} + g^2_{\text{ab}} \\ &+xw_{\text{ab}} + begin_{\text{ab}} + g^1_{\text{ab}} \\ &+xy_{\text{ab}} + g^7_{\text{ab}} + p'_{\text{ab}} \end{aligned} \xrightarrow{\text{slow}} done^{\text{P}} \tag{63}$$
$$done^{\text{P}} + yd \xrightarrow{\text{fast}} yd \tag{64}$$
$$done^{\text{P}} + d \xrightarrow{\text{fast}} d \tag{65}$$
$$done^{\text{P}} + go \xrightarrow{\text{fast}} go \tag{66}$$
$$done^{\text{P}} + g^2 \xrightarrow{\text{fast}} g^2 \tag{67}$$
$$done^{\text{P}} + xw \xrightarrow{\text{fast}} xw \tag{68}$$
$$done^{\text{P}} + begin \xrightarrow{\text{fast}} begin \tag{69}$$
$$done^{\text{P}} + g^1 \xrightarrow{\text{fast}} g^1 \tag{70}$$
$$done^{\text{P}} + xy \xrightarrow{\text{fast}} xy \tag{71}$$
$$done^{\text{P}} + g^7 \xrightarrow{\text{fast}} g^7 \tag{72}$$
$$done^{\text{P}} + p' \xrightarrow{\text{fast}} p' \tag{73}$$
$$done^{\text{P}} \xrightarrow{\text{slow}} done \tag{74}$$
$$2\,done \xrightarrow{\text{fast}} done \tag{75}$$

Post-Loop Cleanup Finally, we reset the system back to its initial state.

$$st + done \xrightarrow{\text{fast}} done \tag{76}$$
$$g^6 + done \xrightarrow{\text{fast}} done \tag{77}$$
$$cyc + done \xrightarrow{\text{fast}} done \tag{78}$$

Absence Indicators

Twenty-five absence indicators are used by the reactions above. They are generated by the method outlined in the paper and omitted here to save space.