

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.

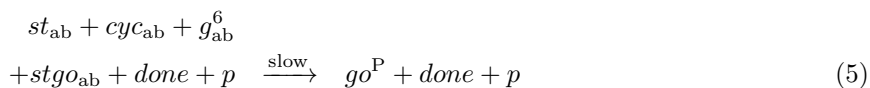
System Initialization We assume that an external source injects some quantity of *begin* at the outset. This type is immediately split into two types, g^1 and g^7 , which will be used to copy x to y (for the line of code $y = x$) and to decrement p (for the line of code $p = p - 1$), respectively. This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



Copy x to y [g^1]



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.



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



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.



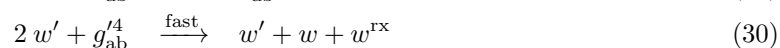
Multiply Loop Start The inner `while` loop is our multiply operation, handled by the next three groups of reactions.



Copy y to d (multiply loop) [g^3]



Decrement w [g^4]



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

$$w_{ab} + w'_{ab} + g_{ab}^2 + xw_{ab} + st_{ab} + done_{ab} \xrightarrow{\text{slow}} g^{5P} \quad (35)$$

$$g^{5P} + w \xrightarrow{\text{fast}} w \quad (36)$$

$$g^{5P} + w' \xrightarrow{\text{fast}} w' \quad (37)$$

$$g^{5P} + g^2 \xrightarrow{\text{fast}} g^2 \quad (38)$$

$$g^{5P} + xw \xrightarrow{\text{fast}} xw \quad (39)$$

$$g^{5P} + st \xrightarrow{\text{fast}} st \quad (40)$$

$$g^{5P} + done \xrightarrow{\text{fast}} done \quad (41)$$

$$g^{5P} + cyc \xrightarrow{\text{slow}} g^5 + cyc \quad (42)$$

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

$$g^5 + y \xrightarrow{\text{slow}} g^5 \quad (43)$$

$$y_{ab} + g^5 \xrightarrow{\text{slow}} \emptyset \quad (44)$$

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 .

$$y_{ab} + yd_{ab} \xrightarrow{\text{slow}} st^P \quad (45)$$

$$st^P + y \xrightarrow{\text{fast}} y \quad (46)$$

$$st^P + yd \xrightarrow{\text{fast}} yd \quad (47)$$

$$st^P + g^5 \xrightarrow{\text{slow}} st + g^5 \quad (48)$$

Set y to d [g^6] Finally, we transfer d to y , clearing d in the process.

$$y_{ab} + g_{ab}^5 + yd_{ab} \xrightarrow{\text{slow}} g^{6P} \quad (49)$$

$$g^{6P} + y \xrightarrow{\text{fast}} y \quad (50)$$

$$g^{6P} + g^5 \xrightarrow{\text{fast}} g^5 \quad (51)$$

$$g^{6P} + yd \xrightarrow{\text{fast}} yd \quad (52)$$

$$g^{6P} + d + st \xrightarrow{\text{slow}} g^6 + d + st \quad (53)$$

$$g^6 + d \xrightarrow{\text{slow}} g^6 + y \quad (54)$$

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

$$p + g^7 \xrightarrow{\text{fast}} p' + g^7 \quad (55)$$

$$g^7 + p_{ab} \xrightarrow{\text{slow}} \emptyset \quad (56)$$

$$g_{ab}^7 \xrightarrow{\text{slow}} g_{ab}'^7 \quad (57)$$

$$2p' + g_{ab}'^7 \xrightarrow{\text{fast}} p' + p + p^{\text{rx}} \quad (58)$$

$$p^{\text{rx}} \xrightarrow{\text{slow}} \emptyset \quad (59)$$

$$p' + p_{ab}^{\text{rx}} + g_{ab}'^7 \xrightarrow{\text{slow}} \emptyset \quad (60)$$

$$2g_{ab}'^7 \xrightarrow{\text{slow}} g_{ab}'^7 \quad (61)$$

$$g_{ab}'^7 + g^7 \xrightarrow{\text{fast}} g^7 \quad (62)$$

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

$$\begin{aligned} & yd_{ab} + d_{ab} + go_{ab} + g_{ab}^2 \\ & + xw_{ab} + begin_{ab} + g_{ab}^1 \\ & + xy_{ab} + g_{ab}^7 + p'_{ab} \xrightarrow{\text{slow}} done^{\text{P}} \end{aligned} \quad (63)$$

$$done^{\text{P}} + yd \xrightarrow{\text{fast}} yd \quad (64)$$

$$done^{\text{P}} + d \xrightarrow{\text{fast}} d \quad (65)$$

$$done^{\text{P}} + go \xrightarrow{\text{fast}} go \quad (66)$$

$$done^{\text{P}} + g^2 \xrightarrow{\text{fast}} g^2 \quad (67)$$

$$done^{\text{P}} + xw \xrightarrow{\text{fast}} xw \quad (68)$$

$$done^{\text{P}} + begin \xrightarrow{\text{fast}} begin \quad (69)$$

$$done^{\text{P}} + g^1 \xrightarrow{\text{fast}} g^1 \quad (70)$$

$$done^{\text{P}} + xy \xrightarrow{\text{fast}} xy \quad (71)$$

$$done^{\text{P}} + g^7 \xrightarrow{\text{fast}} g^7 \quad (72)$$

$$done^{\text{P}} + p' \xrightarrow{\text{fast}} p' \quad (73)$$

$$done^{\text{P}} \xrightarrow{\text{slow}} done \quad (74)$$

$$2 done \xrightarrow{\text{fast}} done \quad (75)$$

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

$$st + done \xrightarrow{\text{fast}} done \quad (76)$$

$$g^6 + done \xrightarrow{\text{fast}} done \quad (77)$$

$$cyc + done \xrightarrow{\text{fast}} done \quad (78)$$

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.