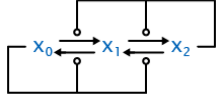
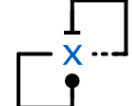
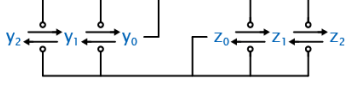
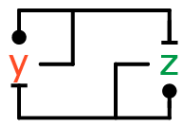


## Additional File 3: Checking some networks morphisms

### Stoichiomorphism & homomorphism from MI to AM

This stoichiomorphism maps  $z, \sim y \rightarrow x$ .

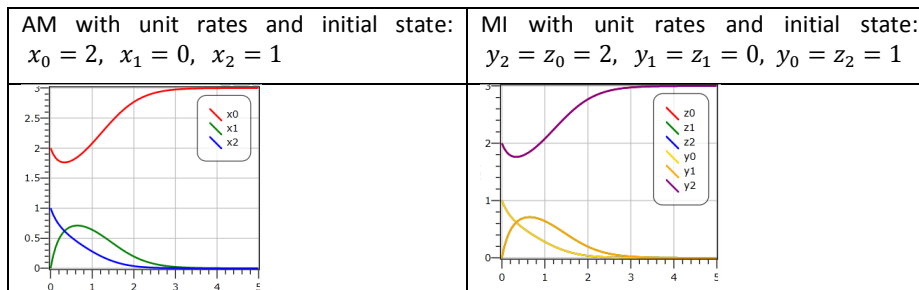
|    | Species                        | Reactions  | Reaction Network   | Influence Network   |
|----|--------------------------------|--|--|---|
| AM | $x_0, x_1, x_2$                | $am_0 = x_2 + x_0 \rightarrow x_0 + x_1$<br>$am_1 = x_1 + x_0 \rightarrow x_0 + x_0$<br>$am_2 = x_0 + x_2 \rightarrow x_2 + x_1$<br>$am_3 = x_1 + x_2 \rightarrow x_2 + x_2$   |  |  |
| MI | $y_0, y_1, y_2, z_0, z_1, z_2$ | $mi_0 = y_0 + z_0 \rightarrow z_0 + y_1$<br>$mi_1 = y_1 + z_0 \rightarrow z_0 + y_2$<br>$mi_2 = y_2 + y_0 \rightarrow y_0 + y_1$<br>$mi_3 = y_1 + y_0 \rightarrow y_0 + y_0$<br><br>$mi_4 = z_2 + z_0 \rightarrow z_0 + z_1$<br>$mi_5 = z_1 + z_0 \rightarrow z_0 + z_0$<br>$mi_6 = z_0 + y_0 \rightarrow y_0 + z_1$<br>$mi_7 = z_1 + y_0 \rightarrow y_0 + z_2$ |  |  |

The species map  $m(s)$  below (outer columns) yields a homomorphism over reactions. We then check that  $m$  preserves net stoichiometry  $\eta(s, r)$ , for all species in MI and all reactions in AM. For example the top left cell checks that  $\eta(z_0, mi_0) + \eta(z_0, mi_4) = 0 = \eta(x_0, am_0)$ .

|                    |       | $m^{-1}(\hat{r}) \subseteq MI$ |              |              |              |               |
|--------------------|-------|--------------------------------|--------------|--------------|--------------|---------------|
|                    |       | $mi_0, mi_4$                   | $mi_1, mi_5$ | $mi_2, mi_6$ | $mi_3, mi_7$ |               |
| $\forall s \in MI$ | $z_0$ | 0                              | 1            | -1           | 0            | $m(s) \in AM$ |
|                    | $z_1$ | 1                              | -1           | 1            | -1           |               |
|                    | $z_2$ | -1                             | 0            | 0            | 1            |               |
|                    | $y_0$ | -1                             | 0            | 0            | 1            |               |
|                    | $y_1$ | 1                              | -1           | 1            | -1           |               |
|                    | $y_2$ | 0                              | 1            | -1           | 0            |               |
|                    |       | $am_0$                         | $am_1$       | $am_2$       | $am_3$       |               |
|                    |       | $\forall \hat{r} \in AM$       |              |              |              |               |

Therefore, by the stoichiomorphism theorem, trajectories of MI that start with

$\forall s \in \{z_0, z_1, z_2, y_2, y_1, y_0\} [m(s)] = [s]$ , coincide with trajectories of AM.



## Stoichiomorphism & homomorphism from QI to MI

This stoichiomorphism maps  $z, r \rightarrow z$  and  $y, s \rightarrow y$ .

|    | Species  | Reactions  | Influence Network |
|----|--|--|-------------------|
| MI | $y_0, y_1, y_2, z_0, z_1, z_2$                               | $mi_0 = y_0 + z_0 \rightarrow z_0 + y_1$<br>$mi_1 = y_1 + z_0 \rightarrow z_0 + y_2$<br>$mi_2 = y_2 + y_0 \rightarrow y_0 + y_1$<br>$mi_3 = y_1 + y_0 \rightarrow y_0 + y_0$<br><br>$mi_4 = z_2 + z_0 \rightarrow z_0 + z_1$<br>$mi_5 = z_1 + z_0 \rightarrow z_0 + z_0$<br>$mi_6 = z_0 + y_0 \rightarrow y_0 + z_1$<br>$mi_7 = z_1 + y_0 \rightarrow y_0 + z_2$   |                   |
| QI | $y_0, y_1, y_2, z_0, z_1, z_2, s_0, s_1, s_2, r_0, r_1, r_2$ | $qi_0 = s_0 + z_0 \rightarrow z_0 + s_1$<br>$qi_1 = s_1 + z_0 \rightarrow z_0 + s_2$<br>$qi_2 = s_2 + y_0 \rightarrow y_0 + s_1$<br>$qi_3 = s_1 + y_0 \rightarrow y_0 + s_0$<br><br>$qi_4 = r_2 + z_0 \rightarrow z_0 + r_1$<br>$qi_5 = r_1 + z_0 \rightarrow z_0 + r_0$<br>$qi_6 = r_0 + y_0 \rightarrow y_0 + r_1$<br>$qi_7 = r_1 + y_0 \rightarrow y_0 + r_2$<br><br>$qi_8 = y_0 + r_0 \rightarrow r_0 + y_1$<br>$qi_9 = y_1 + r_0 \rightarrow r_0 + y_2$<br>$qi_{10} = y_2 + s_0 \rightarrow s_0 + y_1$<br>$qi_{11} = y_1 + s_0 \rightarrow s_0 + y_0$<br><br>$qi_{12} = z_2 + r_0 \rightarrow r_0 + z_1$<br>$qi_{13} = z_1 + r_0 \rightarrow r_0 + z_0$<br>$qi_{14} = z_0 + s_0 \rightarrow s_0 + z_1$<br>$qi_{15} = z_1 + s_0 \rightarrow s_0 + z_2$ |                   |

The species map  $m(s)$  below (outer columns) yields a homomorphism over reactions. We then check that  $m$  preserves net stoichiometry  $\eta(s, r)$ , for all species in MI and all reactions in AM. For example the top left cell checks that  $\eta(z_0, qi_0) + \eta(z_0, qi_8) = 0 = \eta(z_0, mi_0)$ .

|                    |       | $m^{-1}(\hat{r})$        |              |                 |                 |                 |                 |                 |                 |       |        |
|--------------------|-------|--------------------------|--------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-------|--------|
|                    |       | $qi_0, qi_8$             | $qi_1, qi_9$ | $qi_2, qi_{10}$ | $qi_3, qi_{11}$ | $qi_4, qi_{12}$ | $qi_5, qi_{13}$ | $qi_6, qi_{14}$ | $qi_7, qi_{15}$ |       |        |
| $\forall s \in QI$ | $z_0$ | 0                        | 0            | 0               | 0               | 0               | 1               | -1              | 0               | $z_0$ | $m(s)$ |
|                    | $z_1$ | 0                        | 0            | 0               | 0               | 1               | -1              | 1               | -1              | $z_1$ |        |
|                    | $z_2$ | 0                        | 0            | 0               | 0               | -1              | 0               | 0               | 1               | $z_2$ |        |
|                    | $r_0$ | 0                        | 0            | 0               | 0               | 0               | 1               | -1              | 0               | $z_0$ |        |
|                    | $r_1$ | 0                        | 0            | 0               | 0               | 1               | -1              | 1               | -1              | $z_1$ |        |
|                    | $r_2$ | 0                        | 0            | 0               | 0               | -1              | 0               | 0               | 1               | $z_2$ |        |
|                    | $y_0$ | -1                       | 0            | 0               | 1               | 0               | 0               | 0               | 0               | $y_0$ |        |
|                    | $y_1$ | 1                        | -1           | 1               | -1              | 0               | 0               | 0               | 0               | $y_1$ |        |
|                    | $y_2$ | 0                        | 1            | -1              | 0               | 0               | 0               | 0               | 0               | $y_2$ |        |
|                    | $s_0$ | -1                       | 0            | 0               | 1               | 0               | 0               | 0               | 0               | $y_0$ |        |
| $s_1$              | 1     | -1                       | 1            | -1              | 0               | 0               | 0               | 0               | $y_1$           |       |        |
| $s_2$              | 0     | 1                        | -1           | 0               | 0               | 0               | 0               | 0               | $y_2$           |       |        |
|                    |       | $mi_0$                   | $mi_1$       | $mi_2$          | $mi_3$          | $mi_4$          | $mi_5$          | $mi_6$          | $mi_7$          |       |        |
|                    |       | $\forall \hat{r} \in MI$ |              |                 |                 |                 |                 |                 |                 |       |        |

We give an example of how this stoichiomorphism can yield an emulation from QI to MI for heterogeneous rates and initial conditions.

