Inspired by the Oregonator

1 The problem

The *Oregonator* is a mathematical model for a certain class of autocatalytic chemical reactions. The name is a portmanteau of *Oregon* and *oscillator* as the system was developed by Richard J. Field and Richard M. Noyes[1] at the University of Oregon.[2] The underlying chemical reactions are:

$$
\begin{aligned}
A + Y &\rightleftharpoons B \\
X + Y &\rightleftharpoons P \\
B + X &\rightleftharpoons 2X + Z \\
2X &\rightleftharpoons Q \\
Z &\rightleftharpoons fY
\end{aligned}
$$

This was simplified by [Field et al. 1974] where the following set of three coupled differential equations can be found:

$$
\begin{aligned}
\dot{x} &= k_1ay - k_2xy + k_3ax - 2k_4x^2 \\
\dot{y} &= k_1ay - k_2xy + fk_5z \\
\dot{z} &= k_3ax - k_5z
\end{aligned}
$$

This system is then further simplified further,[3] yielding

$$
\begin{aligned}
\dot{x} &= s\left(y - xy + y - qx^2\right) \\
\dot{y} &= \frac{1}{s}\left(fz - y - xy\right) \\
\dot{z} &= w\left(x - z\right)
\end{aligned}
$$

[1]See [Field et al. 1974].

[2]Quite like the *Brusselator*, developed in Brussels, see application note #40, https://analogparadigm.com/downloads/alpaca_40.pdf.

[3]Details are not of interest in the following and can be found in [Field et al. 1974].

with parameters $s = 80$, $q = 10^{-5}$, $w = 0.1$, and $f = 1$.

This already looks nasty (read "stiff"), which is confirmed by a quick numerical experiment showing max$(x) \approx 10^5$, max$(y) \approx 2500$, and max$(z) \approx 3 \cdot 10^4$. This suggests the following scaling factors: $\lambda_x = \lambda_z = 10^{-5}$ and $\lambda_y = 10^{-4}$ resulting in the following system of roughly scaled equations:

$$\begin{aligned}
\dot{x} &= \frac{1}{1000}y - 100xy + \frac{1}{100}x - \frac{1}{100}x^2 && k_{0_x} = 10^3\\
\dot{y} &= \frac{1}{80}z - \frac{1}{800}y - 125xy && k_{0_y} = 10\\
\dot{z} &= \frac{1}{100}x - \frac{1}{100}z && k_{0_z} = 10
\end{aligned}$$

The stiffness shows clearly in the wide spread of coefficients, which are not really practical. This gave rise to some manual experimentation in search of a similar but simpler system, which should also exhibit steep pulses as the Oregonator. The resulting system looks like this with only one really large factor of 100 to be taken care of:

$$\begin{aligned}
\dot{x} &= 0.01y - 10xy + 0.03x - 0.03x^2 && k_{0_x} = 10^3 && (1)\\
\dot{y} &= 0.3z - 100xy && k_{0_x} = 10^3 && (2)\\
\dot{z} &= x - z && k_{0_z} = 10 && (3)
\end{aligned}$$

2 Implementation

The implementation of this system on THE ANALOG THING is straightforward as shown in figure 1. The factor 100 at the y-integrator is implemented by a 10k resistor connected to the summing junction (SJ) of the corresponding integrator on THE ANALOG THING.[4]

The behavior of the system can be either observed directly with an oscilloscope connected to x, y, and possible z or using the Arduino hybrid computer library `THAThc`.[5] Figure 2 shows an oscilloscope screenshot.[6]

[4]Inputs with weight 1 have a 1M resistor in THE ANALOG THING.
[5]See `https://github.com/anabrid/THAThc`.
[6]Due to the rather low repetition frequency of several 100 ms a digital storage oscilloscope was used.

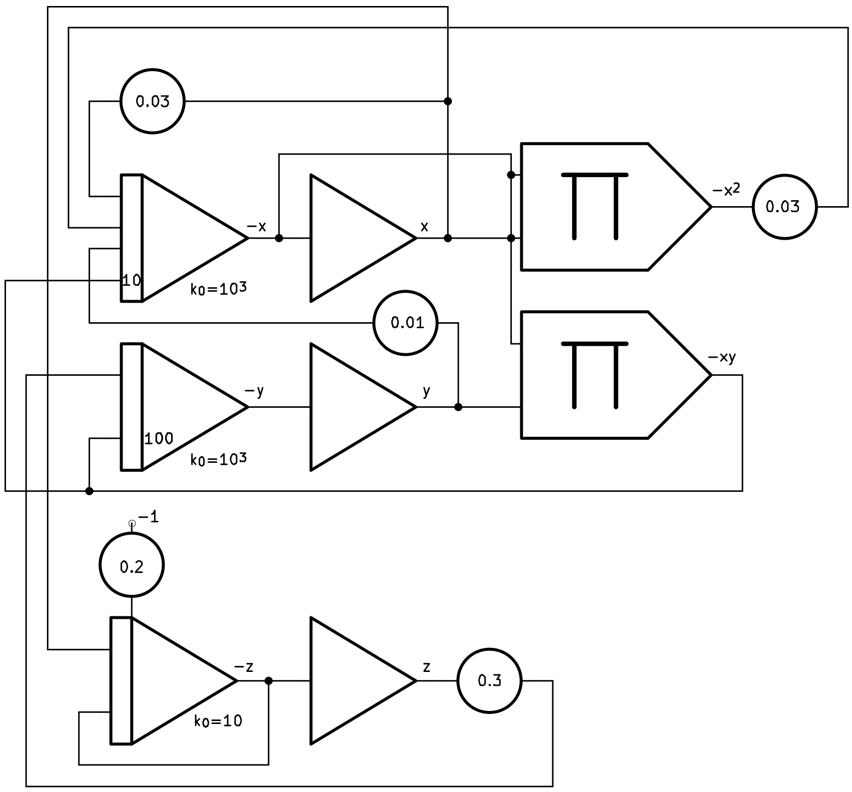

Figure 1: Analog computer program for equations (1), (2), (3)

Using the hybrid computer library it is possible to control THE ANALOG THING from an attached Arduino Mega 2560 and gather data during a run. The corresponding Arduino project is shown in figure 3.

With this program loaded into the controlling Arduino, a single run of the analog computer program with data gathering can be performed by issuing the following commands:

```
optime=1500
ictime=100
```

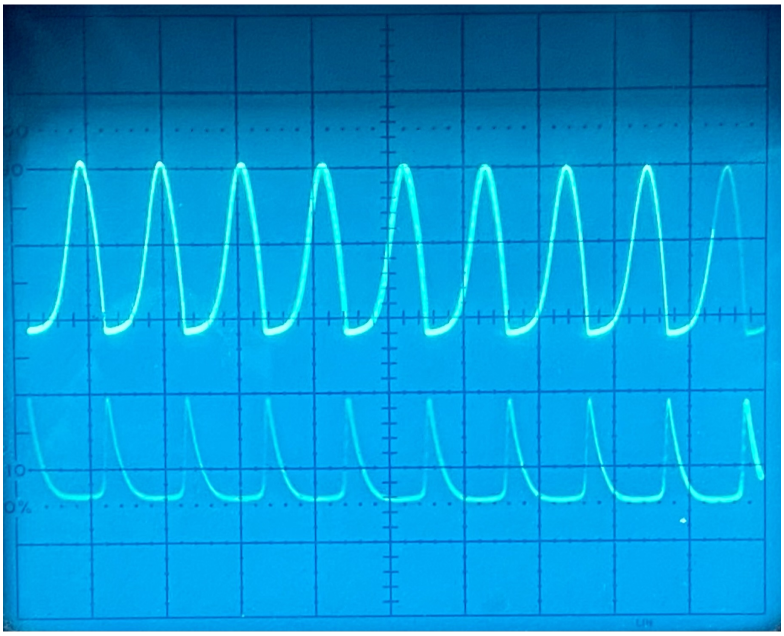

Figure 2: Behavior of the system

```
#include "THAThc.h"
#define BAUD_RATE 250000

void setup() {
  Serial.begin(BAUD_RATE);
  THAThc.begin();
}

void loop() {
  THAThc.shell();
}
```

Figure 3: Arduino control program

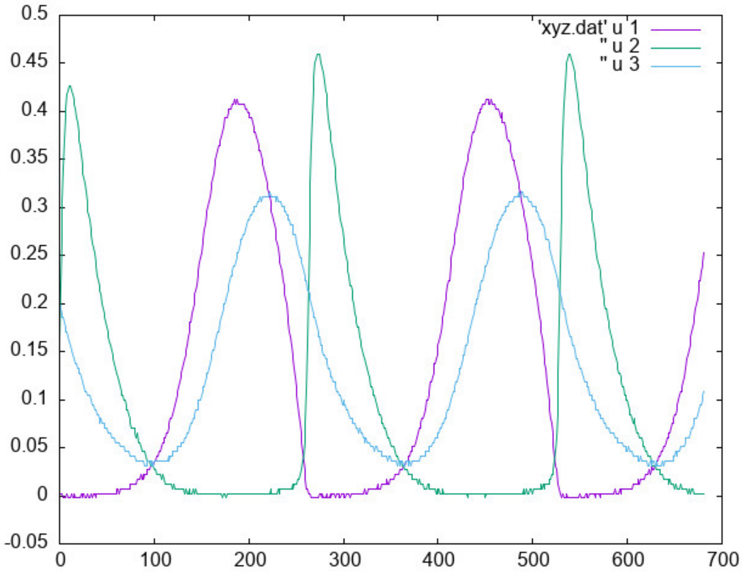

Figure 4: x-, y-, and z-channels captured using the Arduino based hybrid controller

```
channels=3
arm
run
read
```

The `read` command will dump the values of all three channels over the serial line. Then they can be copied from the serial monitor and pasted into a file for subsequent processing. Figure 4 shows a plot generated using `gnuplot`.

Happy analog computing!

References

[Field et al. 1974] Richard J. Field, Richard M. Noyes, "Oscillations in chemical systems. IV. Limit cycle behavior in a model of a real chemical reaction", in *The Journal of Chemical Physics*, Vol. 60, No. 5, 1 March 1974, pp. 1877–1884

[Tyson 1981] John J. Tyson, "On Scaling the Oregonator Equations", in [Vidal et al. 1981, pp. 222 ff.]

[Vidal et al. 1981] C. Vidal et al. (eds.), *Nonlinear Phenomena in Chemical Dynamics*, Springer Verlag, 1981