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Architectural Properties of Bioreactor Embedded Chemical Droplet Computers

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Abstract

Here we present a model and a simulator for a computing architecture that uses excitable chemical droplets, which can be interconnected to form a calculating network. The model uses discrete internal states to represent the excitation phase of each droplet, which can influence the states of neighboring droplets if they are connected. Networks can be analyzed in this framework through simulation and by algebraic probability calculus. Furthermore, it is an abstract, phenomenological model and thus applicable to a variety of implementations for compartmentalized excitable chemical media, such as the Belousov-Zhabotinsky reaction with the right parameterization.

By staying abstract in respect to the chemical implementation, we are focusing on the signal propagation behavior and its implications for possible signal encoding schemes and computing paradigms.

1 Introduction

Chemical computers might be used in many fields of applications, ranging from controlling bioreactors to smart drugs, as reviewed here [4, 5, 17] for example.

In this article, we are focusing on a models and simulations of compartmentalized, excitable chemical media. An excitable medium, for example accommodating the the Belousov-Zhabotinsky (BZ) reaction [7], can oscillate - either spatially or temporally - for many periods while consuming the chemical substrate. When the medium is in the *excitable* regime, it is able to oscillate for one period, once it is stimulated but it will not spontaneously enter a new oscillation phase but return to the quiescent state. Dependent

on the composition of the BZ mixture, other behaviors can be generated but these will not be considered in the approach presented here.

In our case, the medium is compartmentalized into small droplets [15, 1] that form, when the medium is dripped into oil. The compartments are stabilized against merging through lipid molecules that self-assemble at the border between the aqueous and the oil phase. Where two droplets meet, a lipid double layer membrane can be formed that allows the passage of chemical reagents to pass through and to trigger an excitation in the neighboring droplet.

2 Models

2.1 Stochastic Model using Discrete Internal States

We are presenting a model for excitable droplets that is parameterized by the four values a, b, c and λ. A value k_i represents the internal state of the complex Belousov-Zhabotinsky oscillation cycle inside each droplet i. k_i is quantized into $(a + b + c + 1)$ discrete steps here.

Different ranges of values represent the droplet oscillation phases *inactive*, *activated*, *stimulating* and *refractory*. Droplets start in the *inactive* state represented by $k_i = 0$. When they are stimulated from the outside or by another droplet, they switch to state $k_i = 1$, entering the *activated* phase. After a more steps, the droplet will switch from the *activated* phase to the *stimulating* phase that allows the droplet to activate neighboring, *inactive* droplets. b steps later, the droplet switches from the *stimulating* phase to the *refractory* phase, that will not yet be excitable again, but will neither activate neighboring droplets any more. After another c steps, the oscillation finishes, returning the droplet from the *refractory* state to the *inactive* state. In total, this makes a total number of $(a + b + c + 1)$ droplet states.

$$k_i \in \{0, 1, 2, \ .. \ (a + b + c)\}$$

While an *inactive* droplet will stay in the state 0 until it is stimulated by a neighbor or the outside, an excited droplet with its value $k_i \neq 0$, on the other hand, will switch to the next phase $k_i + 1$ after an exponentially distributed waiting time t in dependence on the parameter λ.

$$f_{exp}(t) = \lambda e^{-\lambda t} \quad \text{for} \quad t \geq 0$$

The unit rate parameter λ can be interpreted as the number of events occurring in a time unit, so that the unit of λ is $1/s$. So overall, the traversal of

an individual droplet's excitation states as well as the propagation of signals along a chain of droplets can be described as a Poisson process here. We can vary the level of stochastic perturbation that we want to include in the system. When representing one of the phases introduced above with a larger number of discrete states l, the time needed to cover these l steps becomes very concise, so that the system is almost deterministic. When l is small instead, the variance is much larger. A detailed calculation of this effect is given in Section 2.1.2.

Passing the excitation from one droplet to its neighbor happens instantly and deterministically, when there is a *stimulating* droplet connected to an *inactive* droplet. So this model does not currently include the possibility of an excitation wave vanishing by not getting transmitted to another resting standard droplet. Droplets that show more complex excitation behaviors are discussed in Section 2.2.

Starting from these basic assumptions, we can deduce some parameter dependent macroscopic effects, which will be presented in the following subsections.

2.1.1 Expected "Run Length" in Droplets for Fixed Time

When transmitting information via connected droplet channels or *lanes*, we are interested in the speed of the signal transfer. To begin with, we want to describe the number of droplets n, that a signal travels in a fixed time t. Since the waiting times between state changes are exponentially distributed, the number of internal droplet steps k is given by the Poisson Distribution as:

$$P_{Pois}(X = k) = \frac{(\lambda t)^k e^{-\lambda t}}{k!}$$

$$E[X_{Pois}] = \lambda t$$

$$Var[X_{Pois}] = \lambda t$$

To cover a distance of $n = k/a$ droplets, each of the n droplets will have to perform a internal steps to become active and to excite its neighbor. Hence the total number of covered droplets is given by this distribution:

$$P_{Pois}(X = n \cdot a) = \frac{(\lambda t)^{(n \cdot a)} e^{-\lambda t}}{(n \cdot a)!}$$

Resulting in the mean and variance of $\lambda t/a$.

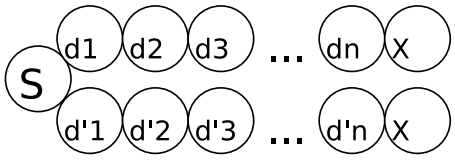

Figure 1: Two parallel lanes of excitable droplets are joined by a common activating droplet S and a common receiving droplet X. In between, both signals are propagated independently. We are interested in the delay between both signals' arrival times at X.

2.1.2 Expected Signal runtime for Fixed Droplet Number

Alternatively, when the time t is fixed, we want to describe the expectation value and standard deviation for the time that is necessary to transport an excitation-signal over $n = k/a$ droplets.

Now we have to use the Erlang distribution, the conjugate to the Poisson distribution, since we are interested in the continuous time density function, describing when the k-th state-changing event occurs.

$$f_{Erl}^{k}(T=t) = \begin{cases} \frac{e^{-\lambda t}\ \lambda^{k}\ t^{k-1}}{(k-1)!}\ ;\ k = n \cdot a & \text{for } t \geq 0 \\ 0 & \text{otherwise} \end{cases}$$

$$E[T_{Erl}] = k/\lambda = \frac{n \cdot a}{\lambda}$$

$$Var[T_{Erl}] = k/\lambda^2 = \frac{n \cdot a}{\lambda^2}$$

So the expected runtime for a distance of n droplets is $\frac{n \cdot a}{\lambda}$. Here again, the runtime is only dependent on the parameters a and λ, not on b or c.

When we would now measure a medium signal runtime t_{real} of a real system, we were free to choose our parameters a and λ, as long as they suffice the equation

$$t_{real} = E[T_{Erl}] = \frac{n \cdot a}{\lambda}$$

By varying the values a and λ now, we can also fit the standard deviation $\frac{n \cdot a}{\lambda^2}$ of the system.

2.1.3 Expected Distance in Runtime between two parallel signals

In order to perform computing operations on the signals, it might frequently be important whether signals arrive more or less synchronously in the setup that is shown in Figure 1. So we calculate the distribution for the unsigned temporal difference τ between two signals that would be started at the same

time $t_0 = 0$ and would be running on parallel lanes along n droplets. To obtain an offset of τ, the first signal arrives at time t, while the later one arrives at time $t + \tau$, $\tau \geq 0$.

Both lanes are statistically independent, so for the probability density of a fixed τ, we integrate the product of both arrival probability densities over all possible arrival times t of the first signal. Then we multiply the product by two, because the temporally first signal can arrive on either of the two droplet lanes:

$$f_{ErlGap}(T = \tau) = \int_0^\infty 2 \cdot f_{Erl}(t) \cdot f_{Erl}(t + \tau)\,\mathrm{d}t \quad ; \quad \tau \geq 0$$

The distribution of gap times peaks at $\tau = 0$ and depends on the number of passed droplets, the length of the *activated* phase a and the phase switching parameter λ. Integrating over all possible τ values times their probability yields the expectation value of:

$$\begin{aligned} E[T_{ErlGap}] &= \int_0^\infty \tau \cdot f_{ErlGap}(\tau)\,\mathrm{d}\tau \\ &= \frac{2\Gamma(k + \frac{1}{2})}{\lambda\sqrt{\pi}\Gamma(k)} \quad ; \quad k = n \cdot a \end{aligned}$$

and analogously the variance of:

$$\begin{aligned} Var[T_{ErlGap}] &= \int_0^\infty (\tau - E[T_{ErlGap}])^2 \cdot f_{ErlGap}(\tau)\,\mathrm{d}\tau \\ &= \frac{2 \cdot (k\pi\Gamma(k)^2 - 2\Gamma(k + \frac{1}{2})^2)}{\pi\lambda^2\Gamma(k)^2} \quad ; \quad k = n \cdot a \end{aligned}$$

where $\Gamma(k)$ is the gamma function, the continuous extrapolation of the factorial function.

2.1.4 Probability for a Signal to Change Direction

Exploring the toy system shown in Figure 2 in simulations, a probably mostly troublesome effect showed up: Signals that propagate along droplet lanes in one direction can spontaneously change their directions, due to variations of oscillation periods between individual droplets.

We assume droplet `d1` from Figure 2 was stimulated by `S`. Basically, the effect shows up when an upstream droplet like `d1`, after activating its neighbor `d2`, becomes *inactive* and thus excitable again, before its neighbor `d2` leaves the *stimulating* phase. Then droplet `d1` enters the *stimulating* phase a second

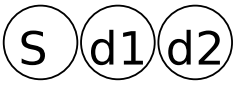

Figure 2: 3 droplets arranged in a short linear lane. The first Droplet `S` is activated externally while the others are activated indirectly: `S` activates `d1`, `d1` activates `d2`. Hence the signal is supposed to propagate from left to right. Nonetheless, there is a parameter-dependent probability that the signal switches its direction, when `d1` leaves the *refractory* state and becomes excitable a second time while `d2` is still exciting.

time and can also activate its other neighbor `S`, inverting the direction of the original signal.

When we consider only two connected droplets, the effect is caused by the process described above. Stochastically, the reactivation of `d1` can happen through two different events: On the one hand, droplet `d1` can return from the *refractory* state while the droplet `d2` is still activating. On the other hand, `d2` might enter the *stimulating* state, while `d1` is already in the *inactive* state. Translating this to probability density functions, we define the following functions:

$$f_{leaveRef}(t) = f_{Erl}^{k=b+c}(T=t) \cdot \sum_{k=a}^{a+b-1} P_{pois}(X=k)$$

and

$$f_{enterStim}(t) = f_{Erl}^{k=a}(T=t) \cdot \sum_{k=b+c}^{\infty} P_{pois}(X=k)$$

to finally calculate the probability for the signal inversion as:

$$P_{Turn}(a,b,c,\lambda) = \int_0^\infty f_{leaveRef}(t) + f_{enterStim}(t)\,\mathrm{d}t$$

While we are still working to find an algebraic expression for the signal inversion probability of longer droplet chains, simulations show that obviously, larger values for the parameter c reduce this effect strongly and that the probability for such an inversion rises, when the droplet chains become longer.

Since the the chemistry of an real system will be constraining the range of the possible parameter concentrations, we can not solely rely on large c values. Additionally the use of building blocks for enforcing the unidirectional signal propagation might be necessary, as discussed in Section 2.2.

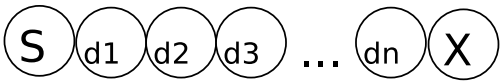

Figure 3: n droplets arranged in a linear lane. The first droplet `S` is continuously stimulated, the output is measured at the droplet `X`.

2.1.5 Emergent Delay Between Consecutive Excitation Signals

When stimulating a lane of droplets continuously from one side as displayed in Figure 3, it might appear as if the maximal signal frequency, the number of excitations that can pass through the lane was simply given by the period length of a single droplet's oscillation. But instead, the frequency of arriving droplets is much lower, even .

The reason for this behavior is

- If we do not include signal diodes to the lane, a signal inversion might occur and destroy the following signal, leading to an doubled output frequency at `X`.
- Even when using signal diodes, one excitation wave can outrun the following wave. In this case, the following signal will die, as it is stopped by the first signal's refractory droplets.
- When the droplets `d1` .. `di` become *inactive* and thus excitable before `di+1` leaves its *refractory* state, the leftmost droplets `d1` .. `di` will start their own oscillation but will be unable to excite `di+1` for a second oscillation. Hence `d` will have to undergo more than one oscillation cycle until the next "real" signal is produced that can pass droplet passing `di`.

2.2 Various Droplet Types

Like specialized electronic components on a circuit board, there might be very specialized droplet types. The "normal" droplets that we were describing so far implicitly represent *or* droplets: when we consider droplet "crossroads" - a droplet that is connected to three or four other droplet lanes - a signal arriving on one lane will spread out in all other directions. Some other droplet types will be introduced in the following.

Starter A very simple droplet that is filled with self-excitatory medium might be used to supply a droplet network with continuous signals, e.g. like a pacemaker or timing signal. It might be generated through a different

BZ medium composition or be externally influencing the droplet, e.g. through optical stimulation.

And Droplets that need at least two active input signals might be build from chemical droplets that contain less excitable BZ mixture. It is an open question, dependent on the further exploration of the droplets in laboratory experiments, how much synchronization between the two input signals is necessary to allow an activation of the 'And' droplet. As an extreme option, no synchronization would be necessary and the activation would be facilitated just by the higher number of signals per unit time.

Repeater To solve the timing problem of the 'And' Droplet, we might assume that we can manufacture a *repeater* droplet that will, once activated, repeat an excitation signal for longer that the typical droplet oscillation period. This might for example be realized through droplets with different medium compositions or with larger radii, as the oscillation period shrinks with larger droplet diameters [14].

Diode Another possibly valuable droplet type might propagate signals only in a single direction while blocking signals arriving from the other direction. It might thus help to insulate some parts of a droplet network from the influences of other substructures or to reduce destructive effects of 'backfiring' signals. A chemical implementation might for example be achieved using diode membrane channels [11] or through differently sized droplets [14] or different media composition.

Inhibition A droplet that inhibits the other droplets, once it is activated itself. One might argue, the oscillation in this droplet might consume the substrate of its neighbor droplets or it might throw its neighbors into the refractory state. We do not yet have a concept of how to produce this droplet type experimentally. So this might be one of the droplet types that are hard to build, we will still consider the implications of the theoretical existence of such a droplet.

3 Simulation Software

3.1 Spatial Simulation Allowing Self-Assembly Systems

We implemented the droplet model that was introduced in Section 2.1 in the spatial, rule-based simulator SRSim [8]. Rule-based modeling is used to investigate - mostly biochemical - reaction networks with a large or even

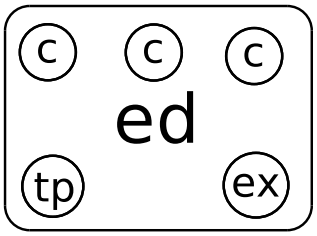

Figure 4: Following the graphical syntax of [6], we show a representation of the elementary droplet of our model here: Here, the droplet contains three times the component `c` that can be used to bind the droplet to other droplets. The component `tp` can be further modified to signal a different type of droplet and the component `ex` is modified to store the oscillation state of the droplet. For the initial, *inactive* state of `ex`, we use the modification tag `~a`. The following letters `~b` , `~c`, .. are used for the following discrete oscillation states.

infinite size of possible reactions and species, based on a limited number of reaction rules. This is for example interesting, when the number of chemical species is large, e.g. when polymerizations happen and each intermediate of the process has to be considered as an own chemical species. In this simulator, we consider a droplet to be a chemical molecule in the simulator. Like biochemical molecules can form bonds and large macroscopic structures, droplet networks are constructed from interconnected BZ-droplets. In this case of droplet computing, each droplet network, which is defined through its connectivity and the individual excitation state of each droplet is considered as a unique molecular species.

The SRSim simulator was developed to add spatial and geometrical features to the rule-based reaction systems by basing it on the molecular dynamics simulator LAMMPS [12]. Though we do not use the spatial features so far, we are already developing the tools to investigate self-assembly scenarios where droplet networks assemble in 3D space from single droplets or from smaller droplet-modules.

The model is specified in the BioNetGen Language (BNGL) [9, 3, 10] by representing each droplet as an *elementary molecule* containing several *components* as displayed in Figure 4. These *components* can be imagined like protein domains with individual functions. Here, they are used to store the droplet's excitation state, to connect it to other droplets and to specify their type.

Once one of the droplets is excited by changing its component `ex` modification from `~a` to `~b`, reaction patterns are defined that make a single droplet cycle through its excitation states until it is finally returned to the *inactive*

state `~a` again. An example of a system investigated with this simulator is given in Section 5.

3.1.1 Input of ASCII drawn Network Structures

While the simulator's asset is basically investigating self-assembling networks, we also added the possibility to import predefined network structures to the simulation run. These structures can than evolve both structurally as well as functionally through the propagation of excitation signals.

The network structures to be imported are declared as ASCII graphs, showing the instances of different droplet types and their connectivity: First the different droplet types are defined, together with a one letter "shortcut-character". Then a 2D map of characters is drawn, where each character is translated into one droplet and where neighboring characters are connected. The number characters `0 - 9` can be used to generate non-planar connections between droplets that are not contiguous or far away in the 2D representation.

An example of a droplet network definition is given in Figure 5.

When the system is imported into the simulator, all droplets are created and the connections are tied. Droplets are initially placed at random positions in the reactor but are drawn together like springs at the connected sites.

3.1.2 Comparison with Stimulation Patterns and Expected Outputs

When we design computing networks from the droplets $d_i \in D$, we probably have some use or function for them in mind. That means we define a number of input $D_{in} \subseteq D$ and output $D_{out} \subseteq D$ neurons that can be stimulated and measured respectively from outside the droplet system. Simplistically, a feed-forward network, which is not using internal states or recurrency, is stimulated at a subset of all input droplets $D_s \subseteq D_{in}$ for some time, leading to a desired measurable activity of a subset of the output droplets $D_{des} \subseteq D_{out}$. In this simple case, a quality measure Q_s for the specified stimulation pattern D_s can be calculated as the minimum number of desired output signals $N_{out}(D_{des})$ received per unit time divided by the maximum number of received but undesired output signals $N_{out}(D_{out} \setminus D_{des})$ of undesired output signals. We clamped the quality values to a range between zero and one by taking the inverse tangent of the fraction and specially treating the case

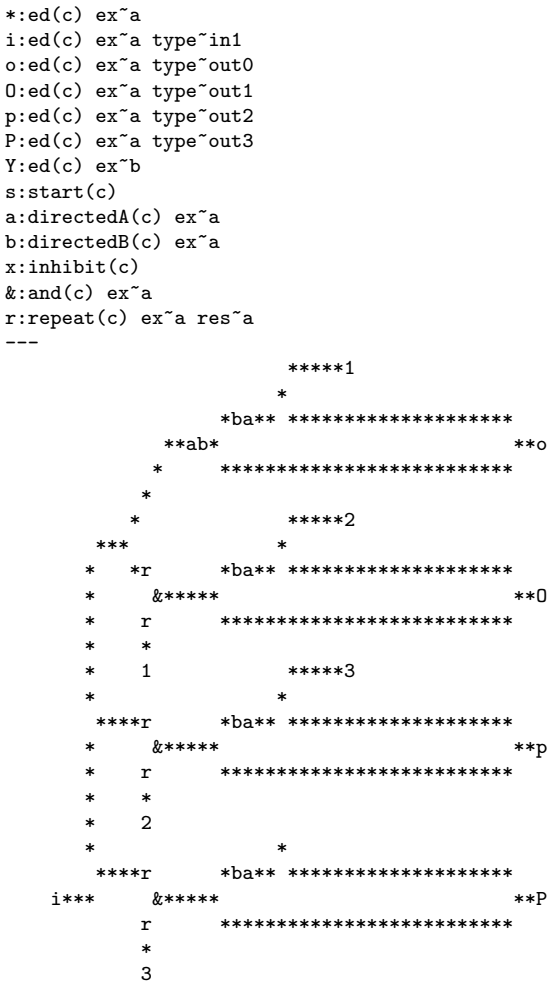

Figure 5: Exemplary network definition as ASCII drawing: each character in the figure represents one droplet; the droplet type is specified by the character; the droplet connectivity is specified by the adjacency in the figure. The network that is displayed here might be used as an input counter. Each input signal `i` at the left activates one of the memory cycles that are connected to the outputs `o`, `O`, `p`, `P`. Only when the first memory cycle is activated, the *and* gate for the next memory cycle be activated by the next input signal. Hence the system is can be triggered through different states.

where no undesired inputs were recorded.

$$Q_s = \begin{cases} 1 & \text{for } \max_{d_l \in D_{out} \setminus D_{des}} = 0 \\ \arctan\left(\frac{\min_{d_k \in D_{des}} N_{t_s}^{d_k}}{\max_{d_l \in D_{out} \setminus D_{des}} N_{t_s}^{d_l}}\right) \frac{2}{pi} & \text{otherwise} \end{cases}$$

Where $N_{t_s}^{d_k}$ is the number of excitation waves passing through droplet d_k in the unit time t_s. When considering the complete set of stimulation patterns S, we can just sum over all stimulation patterns: $Q = \frac{1}{|S|} \sum_{s \in S} Q_s$. Nonetheless, this quality measure will probably still be subject to further investigation when using it to optimize designs for calculating droplet devices.

In the SRSim simulator, we implemented the functionality of declaring stimulations sets S and recording the $N_t^{d_k}$ values as response of the simulated network for each declared output neuron.

When using this evaluation scheme, this implies, that for any droplet module that we are building, we should always guarantee, that there is at least on maximally active output to reference the excitation strength against. If for the correct result of a calculation all outputs should be quiet, we would not be able to differentiate this result from background noise.

4 Signal Encoding Proposals

Clearly, the traveling excitation waves will represent any kind of information that will be processed in droplet networks. But there are many different possible approaches to actually encode information into excitation waves. Also in biological nervous system, different approaches are used, sometimes converted from one representation into another and probably some representations are not even found yet [13, 2, 16]. Though there are probably a lot more possibilities, we will enumerate some approaches, reasoning about consequences of each coding scheme.

4.1 Binary Presence/Absence-Coding on Single Lanes

Probably one of the most straight-forward approaches is to signify binary values through the absence or presence of excitation signals along droplet lanes. When signifying the state `1` by an excitation signal, the `0` signal must be coded by no activity on a droplet. Hence, by principle, we cannot discriminate between no signal at all and the `0` signal. This makes error correction harder in this coding scheme.

Though timing is not used to represent information in this scheme, excitation wave phases might still influence the efficiency of building blocks that depend on more than one input, like *And* or *Inhibition* droplets.

Another problem is negating a signal: A possibility might be to use a *Starter* droplet that will statically generate an active signal that can be inhibited by an input signal. But inhibition on the other hand might turn out to be non-trivial because even when we find a droplet construction to realize inhibition, it will probably be working stochastically such that the inhibitor droplet will block only a subset of the emitted activation waves. Hence, the use of *Repeater* droplets, the construction of parallel inhibitors, averaging the signals or other noise reducing measures might become important here.

4.2 Binary Activity-coding on Two Lanes

Extending the concept of the binary presence/absence coding scheme, we might also add a second droplet lane for the inactive signal, resulting in a $+$ and a $-$ lane. While doubling the number of droplet "cables", this approach has some advantages: To start with, a simple error correction mechanism could assert that the signals on both lanes are not simultaneously active or inactive. Also implementing a negation is perfectly simple now: We only have to exchanging the $+$ and the $-$ lanes. Furthermore, while the *inhibition* type droplet was necessary in the single-lane presence/absence coding scheme to build a negation, the hopefully simpler *and* droplet suffices here for this purpose.

4.3 Phase-and-Reference Coding

Similar to the concept of "temporal coding" in the neurosciences [2], we could also move away from activity coding signals by focusing on the phase of the excitation waves. As explained in Section 2.1.5, the gap between two successive signals is not only explicable by a single droplet's oscillation but emerges from the stochastic deviations of the oscillation phases of many droplets. This delay is probably long in comparison to a single droplet's oscillation phase. Hence we can utilize the expected delay between two signals and code information in the phase difference between two input signals or between an input signal and a reference signal for.

Also with this approach, a signal negation is easily introduced by adding a small number of delaying droplets of half the phase length to a circuit lane.

As we discussed in Section 2.1.3, the delay between two excitation waves will not stay the same when a signal travels longer distances. Hence also the the phase information will degenerate over the distances, which are necessary

to build more complicated networks. Hence micro architectures or modules would be required that could either restore the phase information, or would resynchronize the waves with a dedicated timing signal.

4.4 Rate Coding

In analogy to biological to "rate coding" in biological nervous systems [13], a fuzzy range of values can be encoded in the rate of excitation waves that is sent through droplet lanes per unit time.

As seen in Section 2.1.5, there is an upper bound for the maximum excitation wave frequency. In contrast the lowest possible non-zero excitation rate depends on the examined time window for transmitting information and thus influences the speed and efficiency of computations and signal transmissions.

Possible transformations on droplet signals using the rate coding still need to be elaborated. In any case, it would be possible to transform rate coded signals into activity coded signals on different lanes to further process the signals.

4.5 Pulse-Width Modulation

Please note, that single excitation waves do not posses variable lengths. That is, the shape of a signal can vary stochastically, but the probability distribution for the wave form is given by the physical properties of the droplets chemistry. Different forms of the initial signal do not seem to lead to varying resulting propagating waves. Hence, the Pulse-Width modulation as it is used in telecommunication and microelectronics will probably not be feasible in droplet architectures.

Nonetheless, when larger time frames are considered, the timing between phases of high excitation and phase of low or no excitation might be recognized and could hence be used to code information.

5 Exemplary Systems - A Non-Recurrent Input Number Counter

To test the simulator and the functional evaluation system in the single-lane presence/absence coding scheme, we constructed a simple network that will discriminate between zero, one, two or three inputs that are fed into the system. In response, it should always stimulate one out of four possible output lanes maximally. In this example we used the model parameters

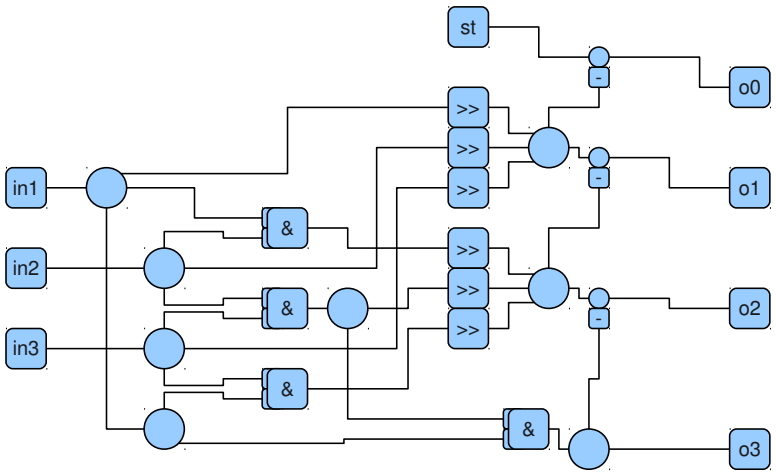

Figure 6: In this schematic circuit diagram, we used different droplet types. On the left hand side, there are the input droplets `in1`, `in2` and `in3` that are stimulated from the outside. These are connected via black lines that represent normal droplet lanes and large circles, that represent *or* droplets - that is, normal droplets that are connected to more than two other droplets, constituting a branching point for an excitation wave. On the right hand side of the diagram, the excitation waves arrive at the output droplets `o0`, `o1`, `o2` and `o3` which are measured by the simulator for the functional evaluation of the network. In between the circuitry, we used the specialized *and*, *diode*, *inhibition* and *starter* droplet types, denoted with '`&`', '`>>`', '`-`' and '`st`' respectively.

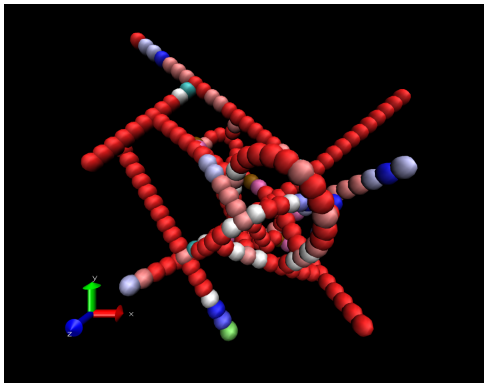

Figure 7: When the droplet system from the schematic circuit in Figure 6 is imported into the dynamic simulator, the structure unfolds as shown here. Different colors correspond to different oscillation states of the droplets. Red colored droplets are *inactive*, while blue droplets are in an excited state. Cyan, white and green droplets are special droplet types and do not show their excitation state here.

$a = 1, b = 3, c = 10$. The parameter λ is not given, since we used arbitrary time units here.

The connectivity of the network is displayed in Figure 6 and leads to the 3d structure of the network that is displayed in Figure 7 when fed into the simulator via an ASCII structure representation, outlined in Section 3.1.1.

Initially, the network is not stimulated externally but excitations from a *starter* type droplet start to stimulate the `o0` output lane for zero inputs. Then, all combinations of one, two and three inputs are fed into the system while recording the system's outputs.

We are currently preparing new simulations that incorporate the new evaluation scheme that is presented in Section 3.1.2. While these new simulations have not finished yet, we are showing a plot using an old evaluation scheme instead in Figure 8.

6 Discussion / Conclusions

In this article, we introduced an abstract, phenomenological model of droplet computation that can be used to investigate stochastic properties of signal propagation, independent on the exact implementation of the droplet chemistry. Through its parameterization, we hope to cover a range of information processing systems built from excitable elements, such as our focused BZ droplets. The model is useful for investigating emergent high level properties

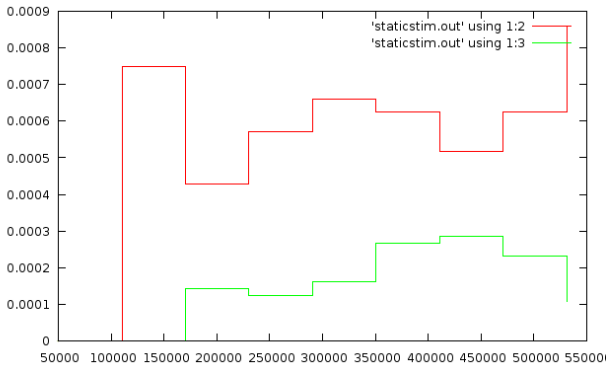

Figure 8: This plot shows the results of a simulation phase in the form of normalized excitations per unit time arriving at at the desired (red) and undesired (green) output droplets. Here, all desired and all undesired output signals are added up, so that the green curve corresponds to the sum of all undesired excitations. Since only one output lane is desired to be active at a time, the red curve is produced by all the signals arriving at this lane in unit time. The first simulation phase up to ca. 110'000 time steps does not show any activity, because here the network was only introduced into the simulator. In the following phases, all combinations of no, one, two and three inputs were fed into the simulator. We can observe, that the number of desired output excitations is higher that the sum of the undesired output excitations for this parameter setting in each of the stimulation settings.

of the signal propagation behavior, that cannot be foreseen from the principle model parameters a, b, c and λ as shown in Section 2.1. Furthermore, a collection of basal droplet types that might contribute to computing modules is introduced in Section 2.2. Additionally we supply a simulator for the described stochastic model and give an example of its use in evaluating and verifying a droplet circuit design.

Following the basal droplet model that is presented here, further steps are necessary to optimally exploit it for the design and engineering of computing networks: First of all, we are currently working to validated with experiments that the model parameters can actually be fitted, such that the model reproduces the observed system behavior. When the basic model is validated, we should search for more specialized droplet types that might perform valuable transformations on excitation signals. For example, droplets utilizing other regimes of the excitable media, such as *sub-excitable* or the *self-exciting* media compositions, might be incorporated into the model for specialized droplet types. There might also be more and better fitting signal encoding schemes that would allow a simpler engineering process, automatic error correction properties or functional redundancies.

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