Molecular computation: a chemist's view

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I am an organic chemist and a big patriot of chemistry. If I never wave a flag it is because I believe that unnatural chemical compounds in the environment pose a bigger danger to humankind and civilization than a horde of terrorists. But chemistry is not just about stinky gooey stuff. It is a unique way to see the world.

The buzz of chemical or molecular computation was at its peak around 2000. For an overview, see [1].

I do not believe in the future of chemical computing based on chemical reactions with DNA or any other molecules. My reason is simple: time. Chemical reactions are not only slow but capricious and sensitive to temperature, solvent, and many other circumstances, the mystique of which constitutes the romantic appeal of chemistry. But I believe in the future of chemical computing of a different nature. Not that I welcome that future with waving a flag, either. And yet the very sound of the words "chemical computation" excites me. Life and mind originated in chemical systems and are based on chemical reactions with capricious portentous biopolymers and their petty but influential entourage.

Here I am presenting my personal attempt to answer the question: **what is mind from the point of view of a chemist?**

All permutations of natural numbers from 1 to 100 are just numbers. They have, so to speak, equal right to exist and do not differ in physical properties for the complete lack of those. Numbers are important but immaterial. This is not so with biopolymers because they fold and coil in various physically different ways. Polymers, unlike numbers, have shape (conformation), mass, and energy. Quite like living forms.

It is the fact that a molecule of a protein computes (or, as a chemist would say in his childish innocence, **takes**) its own shape incredibly faster than the largest computers. This shape is under a powerful influence of the temperature, solvent, and small molecules in it, but in the living cell it is remarkably stable.

The molecule of protein is a linear chain looking like a string of beads of various color and shape, about twenty varieties in all. From a layman's perspective all such strings of 100 beads are the same. In fact, when the molecule twists, coils, and bends over backwards, which it could naturally do in a solution, one hundred beads form and break weak bonds of different strength with each other, as they would do if they were scattered. The string, however, constraints their relative positions, imposing a topology on the interactions. After a while, the molecule finds such a shape which is most stable, i.e., the energy of which is the lowest. This is not so simple, however. Actually, the protein folding exemplifies one of the toughest scientific problems [2].

But why is the problem so complicated?

Note, that if two conformations, as the shape is called, have a close energy, they both will be present in comparable concentrations.

Note also that there are a multitude of factors that may enhance the stability of one form in comparison with another.

Note that the proteins are synthesized sequentially, which significantly restricts the way they can fold.

Note, that we never know whether the natural shape really has the lowest energy. Many, if not all, proteins, actually, fold once and never unfold unless in the test tube.

Note on top that various **time sequences** of shapes can have different probabilities because some forms turn into each other faster than others and you will have an idea of the complexity of the problem, which leads to combinatorial explosion in computation. The time needed to compute a single protein exceeds the age of the universe.

Note, if it is not enough already, that our knowledge of chemistry is still incomplete.

Nevertheless, since around the middle of the last century we have learned something important. Chemistry is a science of time. In a long enough time any chemical system will come to an equilibrium. But no living organism is in equilibrium and no life span is long enough. The way to an equilibrium in the form of skeletal remains starts with death.

We can—not too often nowadays—hear demonstrators chanting "What do we want? A star from the sky. When do we want it? Now!" In chemistry, what you can have now or tomorrow can be very different from what you will have in ten days or ten years, just do some research with wine or whiskey.

Thinking, like winemaking, takes time. Isn't it an exciting observation? I am excited because chemical computing looks to me like a way to natural intelligence which is slow and displays in time. Two people will require different times to solve the same problem, and some will give up. Some scientists waste their best years of life in thinking, not even knowing if the problem has a solution, while less ambitious ones follow the beaten track littered with computer printouts.

Two identical computers will spend exactly the same time for solving any computable problem, which is the best evidence of their zombie-like nature. The word "natural," a buzzword of modern super-pop-sub-culture, often sounded in works on chemical computing.

To use chemistry for natural intelligence is a great idea because molecules are amazingly successful in solving their internal problems and negotiating interactions. For this, however, we do not need any chemical lab.

Figure 1, from [3] illustrates how collisions between particles can be replaced by communication between their immobile proxies. See also [4].

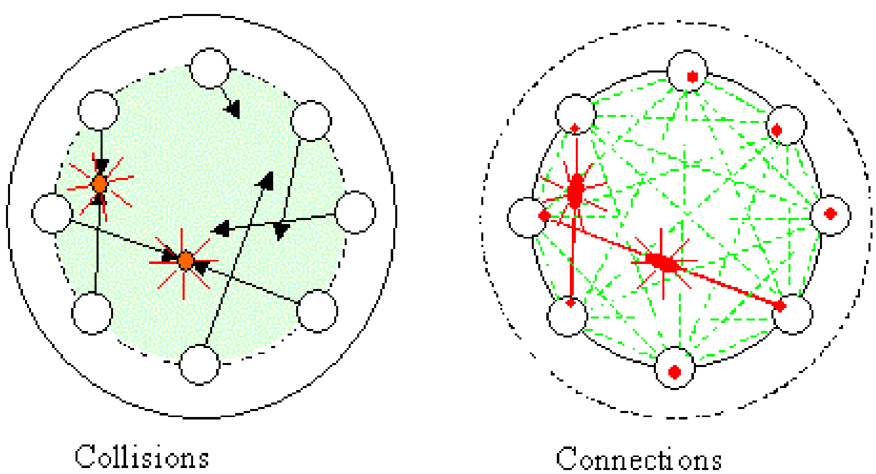

Figure 1. Collisions and connections

What we need is to substitute the interaction of **fixed** atoms for collisions of free atoms. Instead of bumping into each other, let us arrange a kind of marketplace where atoms can locally negotiate with each other whether it is good for them to be connected under the circumstances of the current market and its global indexes, plus the weather and the football scores. Of course, this is something which is possible only if each atom, fixed to its position, is hooked up to a kind of Internet and can contact any other atom, bypassing Wall Street and its not always honest gurus. Let us assign a value **G** to each contact, declare that "good" means the highest value of **G,** and watch how the sum of all such values changes. The market will never come to an equilibrium—weather and the scoreboard change, not to mention any market—but some of its states will have higher **G** than others. A certain topology can be imposed on the market, in which some pairs of atoms are close to each other and some are less close, so that neighbors have preference in communication.

The idea that chemistry is not just about the atoms of Periodic System is relatively new. It was introduced within the framework of Artificial Life. See, for example, [5], from which I quote:

> An artificial chemistry system is a man-made system that is similar to a real chemical system.

"Collision" in an Artificial Chemistry is simply a rule describing the **interaction**.

Collisions can be interpreted in various ways. Thus, in the market economy a transaction can be regarded as collision. A phone call is a collision, too. So is an automobile collision for insurance industry. Triple collisions are relatively rare in both chemistry and on the road. No wonder, stock markets are a popular topic of physics journals.

Artificial chemistry, in my view, misses one fundamental aspect of chemistry: structure. Otherwise, it is a typical science of time, i.e., chemistry. More specifically, the aspects of time in chemistry are called chemical **kinetics,** and artificial chemistry is very good at that. Its "molecules" are always populations. Large numbers are needed for predictability.

I am not going to develop this idea any further because it is not new and I am not pursuing any marketable goods and gains. I am attracted to the beauty and malice of ideas as I am attracted to the beauty and malice of molecules.

My primary intent is to draw attention to the meaning of the term "atom."

What it means to be an atom or a molecule not from the point of view of chemistry and physics, but from the point of view of mathematics? It turns out that there is a mathematical theory of atom-like objects related to molecules, life, mind, society, and their creations. It is Pattern Theory (PT) of Ulf Grenander [6]. As a chemist, I see in it a kind of generalized chemistry which is no substitute for any natural science but is a way to see all natural and artificial structures, from molecules to societies, in a single picture. Unlike Artificial Chemistries, this **mathematical chemistry** is all about structure and, therefore has one important property shared with organic chemistry: you never lose the ability to see the complexity and individuality of the objects. I think this is a beautiful idea. For a non-chemist, all chemical formulas are a visual gibberish. For a chemist, molecules are as individual as friends, relatives, and lovers, falling into ranks and categories, of course. Yours and my enemies are among them, too.

Thereby I suggest a **new** (not sure about that, but be **bold**, be not afraid) form of a quasi-molecular computer (P-Tuter, in honor of Pattern Theory), with appropriate hardware. It consists of a large set of elements that can communicate with each other. It could be done in a wireless (or combined) mode, which, if signals are weak enough, would introduce a topology. The set can be expanded by adding or activating new elements at certain places. Each act of communication is an act of computation. P-Tuter has no program, but it evolves from **infancy** by bootstrapping and growth until **maturity**. This ability to have infancy must be included in the definition of natural intelligence.

This computer will be unable to count and perform mathematical operations, for which a common computer or just fingers can be used, but it might be able to do …what? Thinking? Simulating? Daydreaming? Sleeping?

The answer is, it will be maintaining **homeostasis** or returning to it after being knocked out. Isn't that what we all do with our lives? This is what a molecule of a biopolymer, living cell, developing child, an ecosystem, society, and businessman all do with more or less success.

I do not need to develop this idea either because I know that it is not new. It belongs to W. Ross Ashby, see, for example, [7] , but was practically abandoned, in spite of remaining strong reverence for him, in favor of artificial intelligence which can do anything we want except one small thing: thinking.

The idea that I am trying to explain at least overlaps and probably fits within with the original concept of "chemical reaction model" of Jean-Pierre Banâtre and Daniel Le Métayer [8] and subsequent "chemical abstract machine" (cham) of Gérard Berry and Gérard Boudol [9] and "collision-based computing" of Andrew Adamatzky [10]. Although I recoil from any kind of "wet-ware" and feel uncomfortable with mathematical formalism, I refer to [8-10] as excellent presentations of the most general principles of parallel chemical computation.

> Not being an expert, I see a high degree of parallelism between the original idea [8] and Hopfield nets: full connectedness, cardinality of multisets as weights, and the coming to equilibrium.

I believe, however, that the design of the natural mind could be a particular rather than general case of collision-based computing. .

What is mind from the point of view of a chemist?

My hypothesis is that an individual mind is a system with **a chemistry**, in a generalized sense, **which**, unlike chemical systems, **cannot contain copies** of ideas and their atomic components. I cannot substantiate more than that, but it is a chemistry in which each structure exists in a single copy. Mind is born copy-destroyer. This brings it closer to art: two identical artworks is one work, not two. Thought can be cloned (you never know how exactly) in a different mind, but not in the same.

This vision of the mind dramatically differs form artificial chemistries which study **populations**, i.e. large numbers of almost identical in some aspect copies. It also does not quite resonate with Pattern Theory which silently assumes that if you deal with probabilities you must have large numbers of copies. Well, we can do without copies because the identical events could form statistical ensembles in time. Indeed, the probability of our thinking about dogs during the day assumes such a time series over a much longer time. But the chemistry of mind presupposes that there is only one idea of dog as a species in the mind. Same in biological taxonomy: there is one and only *Canis Canis*, our dear friend.

In the language of mathematics, the mind as a chemistry cannot contain any multisets, for example, **{A, A, B, A, B, B}**. For the mind, it is always **{A, B}**, although it could be { **A,**B } or { A, B }. By its very nature, the mind can hardly count numbers other than very small (two or three?), unless taught so.

As Henri Poincaré noted, mathematics is the way to name many things with one name. Our mind is a mathematical-chemical centaur. For the mind, an atom or a "molecule" of an idea is either **old** or **new**. The **new** atom and new "molecule" can be added to memory. Another such (i.e., **new old = different**) atom may increase the weight of the stored old one, but it does not make another entry into the registry. Mind, like a dictionary, does not duplicate entries. When a chemist draws a formula of a molecule, she does not care whether there is one molecule or one zillion. The formula is an idea. Mind operates with ideas and two identical ideas are just one.

I would use the following illustration of the difference between **metaphoric addition** in mathematics (arithmetic) , physics (mechanics), chemistry, biology, and the science of the mind (cognition).

Math	**1 + 1 = 2**
Physics	**1 + 1 = 1**
Chemistry	**1 + 1 = 1 + 1 , 1 + 1 = 1……1**
Biology	**1 = 1 + 1 , 1 + 1' = 1 + 1' + 1 + 1'**
Cognition	**1 + 1 = 1 , 1 + 2 = 1……2**

Numbers in math do not differ physically, but are labeled differently. In physics, the extensive values are additive: two identical coins weigh twice as much as 1, but they are made of the same stuff. In chemistry, atoms cannot be either added or divided in any way, but can be bonded, whether they are identical or not. The labels never change.

In cognition, as in mathematics, atoms do not have any extensive value and do not change the label if two identical atoms are added. Two different atoms can bond, as in chemistry, but they never change their labels. There is also an intensive value: weight (a very inappropriate term) or intensity, which has parallels in physics. I symbolize it by a darker highlighting.

I emphasize the metaphoric nature of this comparison, but it points to one major difference of the phenomena of the mind (and life as well) : cognitive systems are irreversible in the most profound sense. You can present 2 as 1 +1 in mathematics, but you can never present 1 as 1+1 in cognition, although it happens in biology every minute.

At the same time, the sciences are not separated by stone walls: they are different projections of the only world we have and they are all related.

Otherwise, mind is pure meta-chemistry: atoms of thought (*generators* in PT) combine into molecules of thought (*configurations*).

Such chemistry has been developing over several years in project GOLEM [11]. PT answers the question "what is thought?" in the following way: thought is a configuration, i.e. atomic objects (generators) connected in a particular order. Note, that like in real chemistry and unlike all countless approaches to semantic representations (but not quite unlike neural networks), each atom and each bond in GOLEM's mind have a weight in the form of energy/probability, which changes in a non-equilibrium manner.

The beauty of the idea in my chemical eyes is that Pattern Theory answers the question about thought in exactly the same way as chemistry had answered the question about molecule about a century and a half ago, after which chemistry became science overnight. Instead of inventing various **ways** to write formulas of unobservable molecules, which has been the hobby of many computer scientists and philosophers working on semantic representations, the chemists decided to focus on the questions:

1. Which atoms are connected into a molecule?

2. Which of them are bonded to which and how.

3. What can happen to the bonds?

In the eyes of Pattern Theory thought is a set of atomic objects connected in a particular way. The bonds can break up and lock in a different order. This is also the essence of chemistry, which had become a successful science long before the molecules could be directly observed.

I must acknowledge that neural networks inherited a good deal of the spirit of homeostat. If something carries a serious promise of evolving into natural mind, it is neural nets.

The natural question about the difference between the P-Tuter and neural net of whether simple (Hopfield) or sophisticated (Grossberg and Carpenter) type is difficult to answer in a few words, but I will try. **Figures 1** and **2** illustrate the similarity (which is even stronger in case of Hopfield net) but the major difference is hidden.

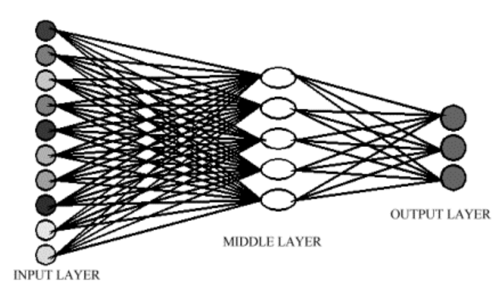

Figure 2. Feed-forward neural net. From [7].

If I am not mistaken, in the absence of input, nothing happens inside any neural net. They are input-output devices, although not always of purely feed-forward kind. In a non-equilibrium chemical system, as well as in the periodically disturbed homeostat, something always happens without any sensible output. Disturbance is not an input in AI sense, either, because it carries no information. It is noise. Cognition is a transition from the world as senseless noise to the world as reasonable order.

The main property of thinking is its spontaneity, or, better, an **unpredictable** and potentially **large** time interval between input and output. Sometimes either input or output is very hard to discover. Besides, thought is absolutely **unobservable**. We can only reconstruct it from verbal output and behavior. We feel that the person lies, we might even detect it physically, but there is no perfectly reliable way to direct the concealed thoughts to the output, or I just don't know about it.

The recurrent neural nets require some post-input processing, but it is predictable (algorithmic, better to say) and, as everything in unnatural computers, observable.

Riding bicycle does not require thinking: reaction is immediate and instinctive. But as soon as the cyclist (state leader) is in an atypical situation, facing a choice between hitting a pedestrian (war) or hitting a tree (dangerous peace), the choice requires thinking, **for which there is no time.** The chemical concept of transition state, paraphrased for the occasion, means that the thinker—**most probably**—will do what can be done faster, i.e., for which the kinetic barrier is lower. This may depend in my example on the thinker's ethics, whose well-being he values more, whether the pedestrian is a child, and how thick the tree is. Transition state in chemistry is an irregular, confusing, and ephemeral structure, as little observable as thought, with more than one exit toward stable states. Thinking in a similar mental state is **subconscious**. When there is enough time, however, all pros and contras can be considered, weighed, and even put to record.

As a chemist brought up in the science of time, I would add to GOLEM only kinetics and the concept of transition state to make a prototype of P-Tuter. The rest are details that can be always worked out along the way to natural intelligence. The inputs and outputs can be attached, but they are not essential. GOLEM thinks in the sense that it does not solve any practical problems by a knee-jerk reaction—quite a paradox, but in fact, the essence of the slow cooking of thinking. Whether you see me or not, *cogito, ergo sum*.

Erwin Schroedinger, answering the "what is life" question, said that it was something we knew (crystal) but with some oxymoronic property (aperiodic). I believe that mind is an **anumeric** (for the lack of a better term …aplethic? think as the opposite of plethora) quasi-chemical system in the sense that it has no countable copies of the same particle. How oxymoronic is that? It sits right on the borderline of moronity . Mind is alive but life is all about **chemical copies** of DNA, the more, the merrier. Alas—and fortunately—not all of them are exact, which makes the idea of **anumericity** (aplethity) not so stupid. Ideas are symbols. Two identical symbols are one. In the society of populations they acquire the power of numbers, as Karl Marx was the first to note, and as we can see at any democratic election.

I must mention briefly another delicate aspect of the mind, which is well visible to a chemist. It is assumed that in a chemical system any molecule can collide with any other. This may be true in an ideal gas system but far from it in a liquid one because of slower diffusion. Neither is it true about Internet. Access to a site can be slowed down or blocked if too many users rush to it. Besides, nobody has either time or need to contact everybody. I don't believe the P-Tuter can use anything like that, especially, if flooded with spam. Fortunately, there is a natural blessing for the mind in the form of competition for energy resource. Life is a chemical process far from equilibrium and this is why it requires constant supply of energy. Firing of neurons is no exception. This is why only a part of them (I don't know how big) can be active simultaneously and they compete for this right. This principle can be compared with a very high gasoline tax that limits consumption, traffic, and even how **large** a car can be. Thinking is heavily taxed.

How can such systems emerge? In a large combinatorial system, it is easy to create something new, unseen, and unheard of. But in a small but fast dynamic system it is impossible: the combinations are easily repeatable within a short time. In large enough combinatorial systems there is no way to **the past**. The property of **novelty** does not apply to small systems. The wonderful properties of life and mind are direct consequences of combinatorial growth. If we want to reproduce **natural** mind, **we must start with small systems**. This powerful principle was clearly stated by Jeffrey Elman

[12], who referred to the earlier **less is more** principle (Elissa L. Newport). This is what I mean by infancy of the natural computer.

Should I better say that mind is an **artist**? Yes, I believe that if there is a homunculus inside the mind, "it" is not only a mathematician, physicist, and chemist, but also an artist who may imitate ready patterns for most of the time, but sometimes rises to the heights of creativity. But haven't I said "past" in the previous paragraph? Then homunculus must be a historian, too. The combination of such talents is the best proof that homunculus does not exist.

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