MOLECULAR FUZZY INFERENCE ENGINES

Development of Chemical Systems to Process Fuzzy Logic at the Molecular Level

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Abstract: Current Information Technology is pursuing a revolution in the design of computing machines: it is trying to pass from macroscopic processors miniaturized through top-down approaches, to microscopic processors made of single molecules assembled through bottom-up approaches. When computations are carried out by single atoms and molecules, quantum logic can be processed. It is difficult to devise a quantum computer due to the decoherent effects exerted by the surrounding environment. However, it is still possible to work out with molecules, by abandoning the lure of quantum logic and processing classical logic. Single molecules make binary computations, whereas ensembles of molecules can be used to implement either Boolean logic gates or Fuzzy inference engines. The behaviours of two chemical compounds after photo-excitation are described as examples of quantum systems whereby Fuzzy logic can be processed by exploiting the decoherent effects exerted by the surrounding microenvironment.

1 INTRODUCTION

Information Technology is trying to develop systems capable of processing larger amounts of information at increasingly high speed and lower power, volume and price. Current computers are based upon semiconductor technology and electrical signals. Their computational power has been growing exponentially. The pace of their improvement is epitomized in the empirical Moore's law, stating that the number of transistors per chip doubles every eighteen months (Jurvetson, 2004). Moore's law has been obeyed, almost precisely, in the last forty years, by virtue of the continuous progress in the miniaturization of computer's processors.

In current computing machines based upon classical physics, both Boolean and Fuzzy logic can be processed. Binary information is recorded in macroscopic two level systems: i.e., when there is no electrical current flowing through a wire, it represents a logical "0", whereas when there is some current flowing through, it represents a logical "1". These two states form a bit of information. All Boolean computations are based on logical manipulation of bits through logic gates acting on wires representing these bits. On the other hand, the most effective implementations of Fuzzy logic have been achieved by the use of analog electronic circuits that are based on continuously variable electrical signals. Boolean binary logic has the peculiarity of manipulating only statements that are true or false, reducible to strings of zeros and ones. However, quite often, the available data and knowledge suffer a certain degree of uncertainty and imprecision, especially when they are based on subjective linguistic statements. In all these cases, it is still possible to process information by abandoning hard computing, based on binary logic and crisp systems, and adopting soft computing, based on Fuzzy logic, neural nets and probabilistic reasoning (Zadeh, 1994). Fuzzy logic is likely to play an increasingly important role in the conception and design of systems whose machine intelligence quotient is much higher than that of systems designed by conventional methods, since it affords to deal with certain and uncertain information, objective and subjective knowledge.

Until now, the miniaturization of computer's elements has been pursued by the top-down approach through photolithography and related techniques. The race towards always smaller dimensions is now approaching some fundamental limits, because processors are being made of a few atoms. Fundamental technological problems arise, such as current leakage and heat dissipation. Therefore, an alternative strategy, named as bottom-

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up approach (Feynman, 1960), has been put forward over the last few years. It is based on the idea of building a computer with its underlying hardware based on single molecules, self-assembled supramolecular entities and/or chemical reaction networks coupled with diffusion processes. The development of molecular logic gates will allow not only electrical but also other physical and chemical inputs and outputs to be exploited. The purpose is to find out molecular systems whereby not only Boolean but also Fuzzy logic can be processed.

2 COMPUTING WITH MOLECULES

Working with single atoms and molecules entails to deal with the laws of the quantum-mechanics, therefore quantum computation can also be carried out. The elementary unit of quantum information is the qubit or quantum bit (Schumacher, 1995). A qubit is a quantum system that has two accessible states, labelled $|0\rangle$ and $|1\rangle$, and it can exist as superposition of them; in other words, a qubit ($|\Psi\rangle$) is a linear combination of $|0\rangle$ and $|1\rangle$:

$$|\Psi\rangle = a|0\rangle + b|1\rangle \tag{1}$$

wherein a and b are complex numbers, and a normalization convention $|a|^2 + |b|^2 = 1$ is generally adopted. A computer based upon qubits promises to be immensely powerful because it can be in multiple states at once. For instance, if it consists of n unmeasured qubits, it can be in an arbitrary superposition of up to 2^n different states simultaneously, differently from a classical computer that can only be in one of the 2^n states at any one time (Bennet, 2000). The superposition can involve also the quantum states of physically separated particles, if they are entangled (Plenio, 2007).

The main difficulty in building a quantum computer comes from the fact that quantum states must constantly contend with insidious interactions with their environment triggering loss of coherence. The superposition state of a qubit, for example $|\Psi\rangle$ defined in equation (1), collapses by decoherence, into a single state, $|0\rangle$ or $|1\rangle$, with probability a^2 and b^2, respectively.

Whenever decoherence effects are unavoidable, the lure of quantum information vanishes. However, it is, anyway, possible to compute with molecules by processing crisp logic. Since a qubit, $|\Psi\rangle$, can collapse into one of two available states, $|0\rangle$ or $|1\rangle$, it seems obvious that just Boolean logic can be implemented at the molecular level.

The ability of making computation by molecules resides in their structures and their reactivity (i.e. affinity). The order, the way the atoms of a molecule are linked, and their spatial distribution rule the intra- and inter-molecular interaction capabilities of the molecule itself, defining its potentiality of storing, processing and conveying information.

Any molecule or supramolecular assembly that can exist in two states of different chemical or physical properties, may be regarded as a potential logic gate if there exist physical or chemical stimuli that can change reversibly the state of the system. Computing with molecules allows multiple inputs and outputs to be used: not only electrical but also chemical, optical, mechanical, thermal, magnetic and other physical ones. The nature of logic gates that can be implemented depends on the response of chemical compounds to the physical or chemical inputs.

When computations are performed through an ensemble of a huge number of molecules, the collective response of the chemical system is continuous on a macroscopic level, although only discrete processes of Boolean character are involved at the molecular level. Whenever the macroscopic input-output relation has sigmoid shape, it has digital character and is suited to process binary logic. For this purpose, it is necessary to establish a threshold value and a logic convention for every input and output variable. The variables can assume simply high or low values that become digital 1 or 0, respectively, in the positive logic convention, whereas the negative logic convention reverses this relationship. On the other hand, whenever the output variable varies smoothly as response of the continuous variation of the input, their relation has analog character and can be exploited to process Fuzzy logic. For this purpose, the entire domain of each variable, referred to as the universe of discourse, is divided into different Fuzzy sets whose shape and position define their membership functions.

Different technological solutions have been put forward for the implementation of chemical computers. They can be grouped in two sets: one that can be defined as based upon "interfacial hardware" and the other that is based upon the so-called "wetware". In the case of "interfacial hardware", the computations are carried out by a single or an ensemble of molecules anchored to the surface of a solid phase (see Figure 1 A).

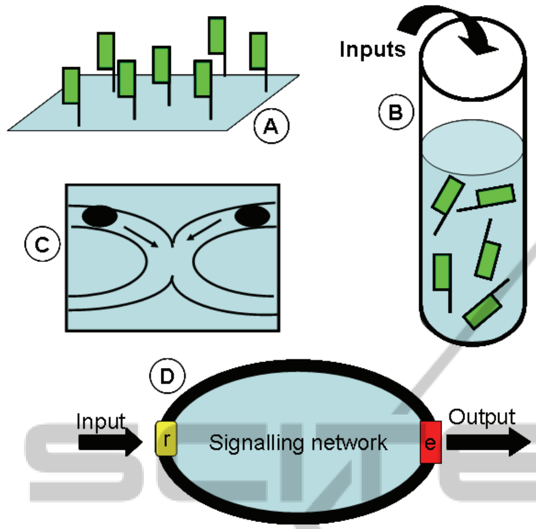
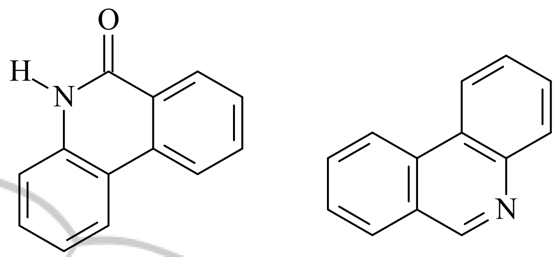


Figure 1: Technological implementations of chemical computing: (A) interfacial hardware; wetware (B) in a test tube, (C) through a microfluidic system, and through a (D) type-cell system wherein "r" stands for receptor and "e" for effector.

In the case of molecular computing based upon "wetware", soups of suitable chemicals process information through reactions, coupled or not with diffusion processes. These soups can work inside a test tube (Figure 1 B) wherein computations are performed through perturbations coming from the outside world. Alternatively, the chemical soups can operate in microfluidic systems (see Figure 1 C) structurally related with the pattern of the current electronic microchips: the microfluidic channels are the wires distributing the information, while logic operations are processed in the reaction chambers. A refined way of implementing chemical logic gates entails emulating the complex molecular signalling circuits that are active inside a living cell (see Figure 1 D). These circuits consist of (i) receptor units, sensing the inputs coming from the outside, (ii) processors, made of reaction-diffusion processes, and (iii) effectors, unveiling the results of computation.

3 CHEMICAL PROCESSORS FOR FUZZY LOGIC

So far many chemical systems have been proposed as digital logic gates (Szaciłowski, 2008), whereas a few have been found suited to implement Fuzzy inference engines. An example of the latter (Gentili, 2007b) is offered by aromatic carbonyl and nitrogen-heterocyclic compounds (see Figure 2), exhibiting Proximity effects in their photophysics (Gentili, 2007a).



(a) (b)

Figure 2: (a) 6(5H)-Phenathridinone, an example of aromatic carbonyl compound, and (b) phenanthridine, an example of nitrogen-heterocyclic compound.

The excitation of these compounds by UV-visible radiation of right frequency triggers the formation of a quantum state, $|\Phi\rangle$, that is the superposition of two pure electronic excited states, as indicated in equation (4):

$$|\Phi\rangle = a|\psi_{\pi,\pi^*}\rangle + b|\psi_{n,\pi^*}\rangle \qquad (2)$$

The two wavefunctions, $|\psi_{\pi,\pi^*}\rangle$ and $|\psi_{n,\pi^*}\rangle$, are relative to the electronic (π,π*) and (n,π*) states, primarily due to the C=O and C=N chemical groups. The $|\Phi\rangle$ qubit has usually a short lifetime, of the order of nanoseconds; therefore, it is not suited to implement quantum computation. $|\Phi\rangle$ quickly collapses to one of its states, $|\psi_{\pi,\pi^*}\rangle$ or $|\psi_{n,\pi^*}\rangle$. If it collapses to $|\psi_{\pi,\pi^*}\rangle$, the molecule can emit light, whereas if it collapses to $|\psi_{n,\pi^*}\rangle$, the molecule does not fluoresce at all, since it relaxes thermally to the electronic ground state bypassing the (π,π*) state. The probability of getting $|\psi_{\pi,\pi^*}\rangle$ is equal to a^2, whereas that of getting $|\psi_{n,\pi^*}\rangle$ is equal to b^2. The coefficients, a and b, depend on the vibronic coupling between the two close-lying (π,π*) and (n,π*) states (Siebrand, 1980). In planar aromatic molecules, such as those of Figure 2, the mode that couples the (π,π*) and (n,π*) states is a low frequency out-of-plane bending mode since n and π orbitals are symmetric and antisymmetric with respect to reflection through the molecular plane (Lim, 1986). The wider the energy gap between the (π,π*) and (n,π*) states, the weaker the coupling between them. When the two electronic excited states couple weakly, the a coefficient of equation (2) assumes large values. That means the probability (a^2) that $|\Phi\rangle$ collapses to $|\psi_{\pi,\pi^*}\rangle$ is high. If a^2 is large, the observable fluorescence quantum yield, measured for an ensemble of molecules, results large.

It is possible to control the extent of the coupling between the (π,π*) and (n,π*) states, and hence the fluorescence quantum yield (Φ_F) of an aromatic carbonyl and nitrogen-heterocyclic compound, by some environmental conditions, such as the temperature and the solvent. In fact, high temperature (T) implies large thermal energy available to the molecular vibrational motions (in particular to the low frequency out-of-plane bending mode, cited above), and hence strong coupling. Moreover, if the lowest excited state occurs to be (π,π*) in character, the energy gap between the (π,π*) and (n,π*) states may increase in going from aprotic to protic solvents, since the (n,π*) state blue shifts, whereas the (π,π*) state red shifts, under the influence of hydrogen bonding. In other words, by choosing solvents with strong hydrogen bonding donation ability (HBD), it is possible to weaken the coupling between the two excited states.

An example of the dependence of Φ_F on T and HBD ability of solvent is shown in Figure 3 for 6(5H)-Phenanthridinone. From the 3-D plot of Figure 3, it is evident that Φ_F varies smoothly with T and HBD ability of the solvent, therefore their relation is suited to process Fuzzy logic. Fuzzy Logic Systems (FLS), based upon the photophysics of 6(5H)-Phenanthridinone, can be implemented. This is due to the fact that the quantum phenomenon of superposition, underlying the Proximity effect of 6(5H)-Phenanthridinone, has characteristics common to the algebra of Fuzzy sets. In fact, the qubit $|\Phi\rangle$, produced by absorption of an UV photon, can be conceived as a Fuzzy variable divided in two Fuzzy sets: $|\psi_{\pi,\pi^*}\rangle$ and $|\psi_{n,\pi^*}\rangle$. $|\Phi\rangle$, which is a superposition of $|\psi_{\pi,\pi^*}\rangle$ and $|\psi_{n,\pi^*}\rangle$, belongs to both Fuzzy sets, at the same time. The degree of membership of $|\Phi\rangle$ to the $|\psi_{\pi,\pi^*}\rangle$ Fuzzy set is a^2, whereas the degree of membership to the other $|\psi_{n,\pi^*}\rangle$ Fuzzy set is b^2. The degree of membership of $|\Phi\rangle$ to $|\psi_{\pi,\pi^*}\rangle$ rules the fluorescence quantum yield for an ensemble of molecules. The values of the degrees of membership of $|\Phi\rangle$ to the two Fuzzy sets can be modulated through external macroscopic parameters, such as T and HBD ability of solvent.

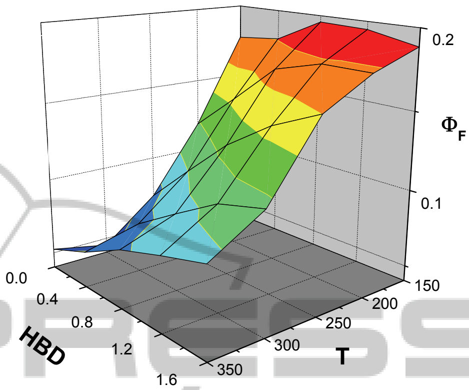


Figure 3: Dependence of the fluorescence quantum yield (Φ_F) of 6(5H)-Phenathridinone on temperature (T) and Hydrogen Bonding Donation (HBD) power of the solvent.

It ensues that FLS can be built by means of this class of compounds with T and HBD ability of the solvent as inputs, Φ_F as output and ultraviolet (UV) radiation as power supply. Through the Mamdani's or Sugeno's methods, the input and output variables are fuzzified, i.e. they are partitioned in Fuzzy sets, defining their related membership functions (μ) and assigning linguistic variables to each Fuzzy set. IF-THEN statements, wherein the multiple antecedents are connected through the AND operator, are fixed as rules. Each Fuzzy rule is interpreted as a Fuzzy implication. Since the antecedent parts of the rules are connected through the AND operator and the cornerstone of scientific modelling, i.e. the cause and effect relation, has to be respected, the membership functions of the rules ($\mu_{R^{(j,k)}}$) are defined only by the minimum (equation 3) and the product (equation 4) t-norms:

$$\mu_{R^{(j,k)}} = \min\left[\mu_{F^j}(T), \mu_{F^k}(HBD), \mu_{F^{j,k}}(\Phi_F)\right] \quad (3)$$

$$\mu_{R^{(j,k)}} = \left[\mu_{F^j}(T)\cdot \mu_{F^k}(HBD)\cdot \mu_{F^{j,k}}(\Phi_F)\right] \quad (4)$$

As the way of determining $\mu_{R^{(j,k)}}$ is fixed, it is necessary to specify how to combine the IF-THEN rules. Generally, they are combined through the t-conorm operator, i.e. the Fuzzy union. The last element of a FLS is the defuzzifier. A criterion for its choice can be based on the attempt of optimising the prediction capabilities that the built FLS exhibit towards the Proximity Effect phenomenon of 6(5H)-phenanthridinone.

Another example of molecular system whereby Fuzzy logic can be processed is offered by tryptophan (Gentili, 2008a). When tryptophan absorbs an UV photon, it passes from the electronic ground state (S_0) to the first excited state (S_1). In S_1 tryptophan is unstable. It decays in a few nanoseconds by following different paths (see Figure 4): it can emit light (fluorescence); it can relax by dissipating the electronic energy in heat (thermal relaxation); it can chemically transform by electron or proton transfer reactions and finally, in the presence of an effective fluorescence quencher, such as flindersine, it can transfer its energy in excess (Gentili, 2008b). These different relaxation pathways are in kinetic competition: the faster the route, the higher the probability of occurring and hence its quantum yield. It is possible to influence the speed of some of these processes and hence the fluorescence quantum yield (Φ_F) through external physical and chemical inputs, such as the temperature (T) and the content of the quencher flindersine. At low temperature and in the absence of flindersine, Φ_F is high. By increasing T, Φ_F weakens slightly since it becomes easier the thermal activated reaction path, i.e. the energy barrier, E_{act}, is more easily overcome (see Figure 4).

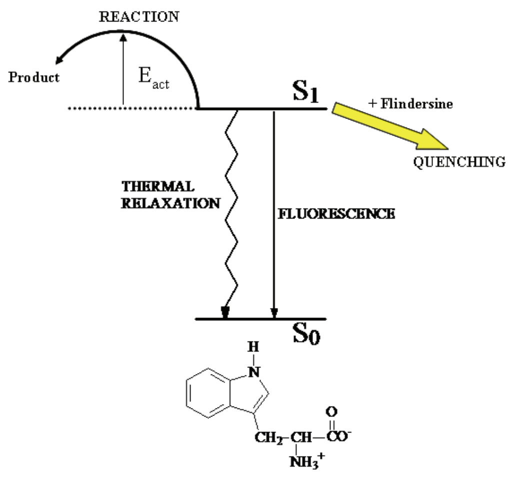


Figure 4: Relaxation dynamics of tryptophan after photo-excitation.

Φ_F is also reduced by adding the quencher flindersine. Since Φ_F varies smoothly with T and the moles of flindersine, it is possible to exploit the photobehaviour of tryptophan to implement Fuzzy Logic Systems (Gentili, 2008a). The temperature and the extent of flindersine act as inputs, UV photons as power supply and Φ_F of tryptophan as output. In ways similar to those explained above for 6(5H)-Phenanthridinone, the macroscopic variables involved are fuzzified; Fuzzy rules, wherein the multiple antecedents are connected through the AND operator, are defined and Fuzzy Inference Engines area started up, based upon the cornerstone of scientific modelling, i.e. the cause and effect relation.

There are also chemical reactions that allow Fuzzy logic to be processed. An example is the biochemical reaction network controlling the glycolysis/gluconeogenesis functions (Arkin, 1994). Here, fructose-6-phosphate (F6P) is interconverted between its two bisphosphate forms by specific kinases and phosphatases. The enzymes in this kinetic mechanism are under the allosteric control of many of the chemical signals of cellular energy status such as cyclic-adenosine-monophosphate (cAMP) and citrate. The dependence of the concentration of F6P on those of cAMP and citrate, gives rise to a 3D surface showing a not abrupt transition from low to high values, such as that of Figure 3. The profile of the 3D surface has a smooth hyperbolic shape and not a steep sigmoidal response: it is suited to process Fuzzy logic.

Another example of a Fuzzy chemical reaction is DNA hybridisation wherein two single-stranded DNA molecules (oligonucleotides) bind to form a double stranded DNA duplex. At room temperature, the hybridisation reaction is not a two-state, all or none process, but it is inherently Fuzzy because it is a continuum of outcomes (Deaton, 2001). The pairs of oligonucleotides formed inside a test tube cannot be divided into distinct sets of hybridised and unhybridised species, but each molecule would have a degree of membership in both.

The best implementations of Fuzzy Logic Systems are human senses, that have to be mimicked by Information Technology in order to reach high intelligent quotients in artificial intelligence. Sight, hearing, taste, smell and touch are inherently fuzzy. They fuzzify the crisp inputs coming from the outside and send the information to the human brain, that is a Fuzzy inference engine, capable of facing up problems based on subjective or imprecise knowledge. Senses are based on a discrete number of perceiving cells acting as Fuzzy sets (Gentili, 2009). For example, in the case of colour perception, we have three types of cones, whereby we distinguish colours: one cone absorbing mainly the blue portion of the visible spectrum, another absorbing mainly the green and the third principally sensitive to the red. Their absorption spectra in the visible, can be conceived as Fuzzy sets, having Gaussian shape: one centred at 437 nm, the other centred at 533 nm and the third centred at 564 nm. When a radiation, having wavelengths included in the visible, hits the retina of our eyes, it activates the three cones in a specific proportion, i.e. it will have specific values of membership functions in three Fuzzy sets. Each combination for the values of three membership functions will be transduced into the perception of a specific colour inside our brain.

4 CONCLUSIONS

Computers of the future will probably consist of molecular processors. Atoms and molecules process quantum logic. However, the insidious actions of the environment trigger detrimental decoherent effects on the qubits. If decoherent phenomena acting on the qubits are unavoidable, it is still possible to compute with molecules by abandoning the lure of quantum logic and processing classical logic. When computations are carried out by single molecules, only Boolean logic gates can be implemented. When computations are performed through a huge collection of molecules, both Boolean and Fuzzy logic can be processed. If the input-output relations are abrupt and they have sigmoidal shape, they are suited to implement binary logic gates. If, on the other hand, the output varies smoothly with the inputs, their relation become suited to implement Fuzzy inference engines. Photo-responses of molecules such as 6(5H)-Phenanthridinone and tryptophan can be used to realize Fuzzy Logic Systems wherein the multiple antecedents are connected through the AND operator. New chemical systems have to be found to process complete Fuzzy Inference engines. They will be implemented by following either the strategy of the “interfacial hardware” or that of “wetware”. The possibility of processing Fuzzy logic at the molecular level will allow high quotients to be within reach of the Artificial Intelligence.

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