PHILOSOPHY AND SYNERGY OF INFORMATION

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Philosophy of Information, like any other part of mankind's intellectual achievements, needs to be written and rewritten in terms of what is of importance to present-day intellectuals. Developments in other areas such as medieval epistemology, or phenomenology and hermeneutics provide some of the problems that have had to be thought through, as well as using historical materials as guides and aids. These proposed explanations provide new lenses or studying and interpreting the past, and this revised version of the past then provides some new ways of looking at the Philosophy of Information at the present. However, it presumes to deal with problems that have had various expressions since even ancient times. The history of Philosophy of Information does not describe a simple linear progression from Plato and Aristotle to our present intellectual situation. Aristotle begins his treatise on metaphysics with the assertion that all human beings have the desire to acquire knowledge, have information: "all men by nature desire knowledge" [1]. By this, he meant that people value knowledge, information for its own sake, entirely apart from its helpfulness. Aristotle mentions the delight in sense perception and in particular, in vision, the sense that distinguish the largest number of comprehensible forms. His teacher, Plato, expressed the enjoyment in vision in a still more radical way in the *Symposium* by attributing it to demonic force, Eros, which raises human beings up from the world of everyday life to the domain of pure intelligible structure. In these two great founding fathers of the Western philosophical tradition, one sees a poetical and a sober or prosaic statement of the universality of philosophical worship.

Inherent in both philosophers, but perhaps more clearly in that of Plato, is the claim that we desire not merely knowledge, in the sense of a system of true proportions about the world but a kind of knowledge that satisfies people most essential desire for happiness or sacredness. In the mythical language of the doctrine of Eros, human beings strive for a completeness of sexual love. Otherwise, stated, sexual love desires the satisfaction of the body, of which the most radical form is the overcoming of personal finitude trough the act of procreation, whereas the love of the soul can be satisfied only through a vision of the order of the whole of human existence.

Platonic dialogues present us with the poetical account of the philosophical nature of the human being. They also raise the question: what kind of knowledge and information is characteristically philosophical? The same questions lie in the heart of philosophical thoughts in different historical times.

In the Greek texts, the philosophical taste seeks to replace opinion with knowledge. Plato and Aristotle both place general truth higher than particular ones, and they define knowledge, information and wisdom in the strict sense as precise and unchangeable.

The word *philosophy* is of Greek origin and means literally "love or friendship for wisdom." This simple linguistic fact shows that philosophy is a central expression of human nature. The popular use of the term philosophy is evident from the fact that wisdom refers traditionally to a kind of general intelligence or capacity for judging effectively in diverse circumstances.

The theory of knowledge otherwise known as Epistemology is best understood in the light of its history. The history involves several traditions. The source of more than one of them can be witnessed in one of the most remarkable passages in the philosophical literature, in Plato's *Meno*.

Epistemology begins from this sense of wonder at the powers of the human information-seeking mind. Meno's slave boy episode marks the beginning of two traditions in epistemology. On one hand, it demonstrates the idea that there is an area of truths that are independent of experience and therefore reachable by pure thinking alone, known as priory truths. On the other hand, there is another line of thought about knowledge and information. How do we reach knowledge and get information? This suggests that the right method of reaching new information and knowledge is by raising the right questions. This idea is even set in the vocabulary in that the English word *inquiry* means “the action of seeking for truth, knowledge or information” (Oxford English dictionary)

The Socratic idea of knowledge/information seeking as questioning was developed by Plato into a method of philosophical training by means of questioning games. These games were studied and systematized by Aristotle, who therefore became the first systematic epistemologist, as well as the first logician and informatist in the Western tradition.

A large body of Aristotle’s writings has come down to us, but unlike Plato’s this *Corpus Aristotelicum* consists mostly of texts in which the philosopher presents his own ideas. Instead of one “knowledge” (episteme) sought by Socrates of Plato’s dialogues and his single method of dialectic, Aristotle distinguishes many “sciences” (epistemai) and different appropriate methods. Aristotle intended to construct a comprehensive system of knowledge, organizing and classifying the sciences into three types-theoretic, practical, and productive-that are distinguished not only by different subject matters but also by different aims, methods, and principles.

Information applies to facts told, read, or communicated that may be unorganized and even unrelated. The term information comes from classical Latin and means to give form or shape to something, to denote the pictorial representation of objects in the human mind, and forming the mind through knowledge, information and communication. Information is a concept situated in the field of human language and intersubjectivity. It refers to the process of telling something to somebody and to the content being transmitted.

Nowadays the concept of information is very difficult to define as it is used in many different areas, not only in philosophy but also in the natural and social sciences. This confusing situation can be considered as an indication of its theoretical application to social epistemology, semantics, rhetoric, information science, library science, information ethics, and cybernetics. Phenomenology studies the structure of various types of experience ranging from perception, thought, memory, imagination, emotion, desire, to bodily awareness, embodied action, and social activity, including linguistic activity.

The medieval concept of *informatio* is presented in Thomas Aquinas'(1225-1274) theory of knowledge and lie in his general agreement with the principles of Aristotle’s philosophy, his conviction that philosophy must be defended and debated on philosophical grounds, and that Aristotle’s philosophy could serve as a solid instrument for a Christian understanding of the worlds, even though Aristotle was certainly not a Christian thinker.

When Aquinas searched for the sources of humanity’s knowledge of sensible objects in question ten of his Disputed Questions on Truth [2]**,** he rejected the theories of the Platonists and Avicenna, since for them sensible objects themselves in no way cause the knowledge we have on them. He likewise rejected the thirteenth century Augustinian theory according to which first a person’s sense power undergoes some impression made upon it by the likeness of sensible object, and then a higher part of the soul by its own action makes itself become similar to the effect made on the sense.

For Aquinas, a proper understanding of Augustine’s illumination theory does not involve an illumination distinct from the light of our intellect: ”the intellectual light itself which is in us is nothing else than a participated likeness of the uncreated light” [3]. God has given to humanity an intellect that enables it to abstract from sense the unchanging or essential elements that are found in sense objects. Aquinas claims to follow Aristotle rather than Plato, Avicenna or thirteen century Augustinians.

Therefore the position of the Philosopher seems more reasonable than all aforementioned positions. He contents that the knowledge of our mind comes partly from within and partly from without, and according to this; it is true that the mind gets its knowledge of sensible objects from sensible things; even though it is the soul itself that forms the likenesses of things in itself. For, it does so insofar as the forms abstracted from sensible things are made intelligible actually by the light of the agent intellect, so that they can be received in the possible intellect.

The Latin term *informatio* became a *terminus technicus* in medieval epistemology and ontology and played an important role in the rationalist and empiricist theories of knowledge of modern philosophy. Since the seventeenth century epistemology has been one of the fundamental themes of philosophers, who were necessarily obliged to coordinate the theory of knowledge with developing scientific thought. Réné Descartes and other philosophers (e.g., Baruch Spinoza, G. W. Leibniz, and Blaise Pascal) sought to retain the belief in the existence of innate (a priori) ideas together with an acceptance of the values of data and ideas derived from experience (a posteriori). This position was basically that of *rationalism* . Opposed to it later was *empiricism*, notably as expounded by John Locke, David Hume, and John Stuart Mill, which denied the existence of innate ideas altogether. The impressive critical philosophy of Immanuel Kant had enormous effects in an attempt to combine the two views. As we can see this dialogue between epistemology and information science, which began fairly recently has a long tradition with regard to the concept of information. Information is familiarly related to concepts such as: to reason with somebody, to listen to what somebody has to say, to a messenger and to his message. There is a context of ignorance and expectation but also of common knowledge to which the information is supposed to be significant. Information is a concept situated in the field of human language and intersubjectivity. It refers to the process of telling something to somebody and to the content being transmitted.

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There is a multiplicity of examples of how phenomenological resources have been used to understand information more generally and information technology more specifically. One might claim that all of these phenomenological studies share at least the underlying view that information and society co-embrace each other by being each other's joint and ongoing condition or possibility for being what they are. As such, they continually draw on each other for their ongoing sense or meaning. One must start by saying that there is not a unified phenomenological approach to information or information technology as such. There is not even a unified phenomenological approach as such. The term ‘phenomenology’ is often used to cover wide units of related approaches that share some common characteristics but not all. *The Oxford English Dictionary* presents the following definition: "Phenomenology. a. The science of phenomena as distinct from being (ontology). b. That division of any science which describes and classifies its phenomena. From the Greek *phainomenon*, “appearance." In philosophy, the term is used in the first sense, amid debates of theory and methodology. In physics and philosophy of science, and information the term is used in the second sense, albeit only occasionally.

The historical movement of phenomenology is the philosophical tradition launched in the first half of the 20th century by Edmund Husserl, Martin Heidegger, Maurice Merleau-Ponty, Jean-Paul Sartre. In that movement, the discipline of phenomenology was prized as the proper foundation of all philosophy. Husserl aimed to pioneer a science of phenomenology that would produce objectively and universally valid knowledge and information. Such scientific and philosophical knowledge would permit us to create science that unifies all existence. Philosophy would be able to fulfill its historic mission: the achievement of pure and absolute knowledge.

Phenomenology studies the structure of various types of experience ranging from perception, thought, memory, imagination, emotion, desire, to bodily awareness, embodied action, and social activity, including linguistic activity. A clear conception of phenomenology awaited Husserl's development of a clear model of intentionality [4]. Husserl would then promote the radical new science of phenomenology, and alternative visions of phenomenology would soon follow. The structure of these forms of experience typically involves what Husserl called "intentionality", that is, the directedness of experience toward things in the world, the property of consciousness that it is a consciousness of or about something. According to classical Husserlian phenomenology, our experience is directed toward — represents or "intends" — things only through particular concepts, thoughts, ideas, images, etc [5]. These make up the meaning or content of a given experience, and are distinct from the things they present or mean.

The diversity of traditional phenomenology is apparent in the Encyclopedia of Phenomenology [6], which features separate articles on some seven types of phenomenology. (1) Transcendental constitutive phenomenology studies how objects are constituted in pure or transcendental consciousness, setting aside questions of any relation to the natural world around us. (2) Naturalistic constitutive phenomenology studies how consciousness constitutes or takes things in the world of nature, assuming with the natural attitude that consciousness is part of nature. (3) Existential phenomenology studies concrete human existence, including our experience of free choice or action in concrete situations. (4) Generative historicist phenomenology studies how meaning, as found in our experience, is generated in historical processes of collective experience over time. (5) Genetic phenomenology studies the genesis of meanings of things within one's own stream of experience. (6) Realistic phenomenology studies the structure of consciousness and intentionality, assuming it occurs in a real world that is largely external to consciousness and not somehow brought into being by consciousness. (7) Hermeneutical phenomenology studies interpretive structures of experience, how we understand and engage things around us in our human world, including others and ourselves. This is another inheritance from Husserian phenomenology that is at the core of hermeneutical theory and is the notion of the life-world and what Heidegger was to call being-in-the- world.

The methods and characterization of the discipline widely debated by Husserl and his successors continue to the present day. Phenomenology as a discipline has been central to the tradition of continental European philosophy throughout the 20th century, while philosophy of mind has evolved in the Austro-Anglo-American tradition of analytic philosophy that developed throughout the 20th century.

In line with the essentials of the “phenomenological method,” hermeneutics is chiefly a descriptive discipline, not a prescriptive one; hermeneutical theory is not a “speculative” nature but is rather an attempt by means of reflection to establish what actually occurs or has occurred wherever we claim to have arrived at an understanding of anything whatsoever (“truth”).

The name of Hermes, the messenger of the Greek gods, gave rise to *hermeneuein,* ‘to interpret” to “art of interpretation.” Hermeneutical theory as elaborated by Hans-Georg Gadamer [7] is usually referred to as “philosophical hermeneutics.” this is an altogether appropriate term in that it points to the feature that serves mainly to differentiate the approach taken to hermeneutics from that of earlier theorists. With the publication of "Truth and Method", hermeneutics is in fact transformed from a specialized method into a general philosophy that sets as its goals the working out a general theory of human understanding itself in all its various forms. In this sense, philosophical hermeneutics corresponds in a rough way to what modern philosophy understood by "epistemology," the general theory of "knowledge and information." As Gadamer stated:" I did not wish to elaborate a system of rules to describe, let alone direct, the methodological procedure of the human sciences….. My real concern was and is philosophic: not what we do or what we ought to do, but what happens to us over and above our wanting and doing". What above all makes Gadamer's hermeneutics actually philosophical is the universal scope and function to which it lays claim. Philosophical hermeneutics, Gadamer says, "takes as its task the opening up of the hermeneutical [interpretive] dimension in its full scope, showing its fundamental significance for our entire understanding of the world and thus for all the various forms in which this understanding manifests itself"[8].

It is important in this connection to note that philosophical hermeneutics as elaborated by Gadamer grows out of and is the continuation of phenomenology as developed by Husserl and Heidegger. Husserl sought to discover for philosophy the same certainty that he found in mathematics. An entry in his diary in 1906 reads: "I have been through enough torments from lack of clarity and from doubt that waves back and forth….one need absorbs me: I must win clarity else I cannot live; I cannot bear life unless I can believe that I shall achieve it."

At the very heart of philosophical hermeneutics is "an entirely different notion of knowledge and truth, as Gadamer puts it. When the philosopher speaks of truth, he generally means openness: "the truth of experience always contains an orientation towards new experience".

In the late 1960s and 1970s, the computer model of mind set in, and functionalism became the dominant model of mind. Functionalism is the doctrine that what makes something a thought, desire, pain (or any other type of mental state) depends not on its internal constitution, but solely on its function, or the role it plays, in the cognitive system of which it is a part. More precisely, functionalist theories take the identity of a mental state to be determined by its causal relations to sensory stimulations, other mental states, and behavior [9].

On this model, mind is not what the brain consists in (electrochemical transactions in neurons in vast complexes). Instead, mind is what brains do: their function of mediating between information coming into the organism and behavior proceeding from the organism. Thus, a mental state is a functional state of the brain or of the human (or animal) organism. More specifically, on a favorite variation of functionalism, the mind is a computing system: mind is to brain as software is to hardware; thoughts are just programs running on the brain's "wetware". Since the 1970s the cognitive sciences — from experimental studies of cognition to neuroscience — have tended toward a mix of materialism and functionalism. Gradually, however, philosophers found that phenomenological aspects of the mind pose problems for the functionalist paradigm too.

One of the great advantages of functionalism is that it allows the mind to be modeled by computers. Once it was understood that any type of system, whether animate or not, could be described in functional terms, it obvious that the analysis applies to computers. A computer is actually an information processor, which is what many philosophers contend a human being. In a computer, the software (the program) functions like the human mind. It reads to external inputs via the hardware and gives rise to certain outputs. The hardware/software distinction thus provides an ideal model for how functionally equivalent elements at a higher level can be implemented by different physical systems at a lower level. One and the same program can be realized by different physical hardware systems; accordingly, it was augured one and the same set of mental processes can be manifested in different forms of hardware implementations.

Functionalism, as a philosophical vanity, was the source of an examination program in cognitive science called" Strong Artificial Intelligence"(Strong AI), which claims that having a mind is simply having a sort of program. This view is also called "Turing-machine functionalism" because it satisfies a test developed by the mathematician Alan Turing(1912-1954) for deciding whether a given system exhibits intelligence or not.

Technical AI is emerging today, and its every advance will speed the technology race. Artificial intelligence is but one of many powerful technologies we must learn to manage, each adding to a complex mixture of threats and opportunities.

AI systems with access to nano quantum machines will perform many experiments fast. They are designing devices in seconds, and replica assemblers are building it without countless delays. Regardless all the experimentation delays, automated engineering systems are moving technology forward with the very high speed.

There is a general notion of what information is and may have dealt with both precise and imprecise information, how information can be quantized, and measured as amount in a variety of situations. Information behaves in accordance with Nature general laws [10].

The Second Law of Thermodynamics deals with physical systems, and also with information processing in natural and engineered systems. The Second Law may well be one of science's most glorious achievements, but as traditionally taught, through physical systems and models such as ideal gases, it is difficult to appreciate at an elementary level. On the other hand, the form of the Second Law that applies to computation and communications is more easily understood, especially today as the information revolution is getting under way.

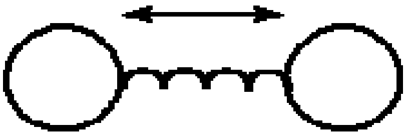
The analogy between information and energy is visible and interesting [11]. Energy as information can be conserved – despite its being moved, stored, and converted, at the end of the day there was still exactly the same total amount of energy. In the context of thermodynamics, this conservation of energy principle is known as the First Law. It has proven to be so important and fundamental that whenever a "leak" was found, the theory was rescued by defining a new form of energy. One example of this occurred in 1905 when Albert Einstein recognized that mass is a form of energy, as expressed by his famous formula $E = mc^2$. That understanding later enabled the development of devices (atomic bombs and nuclear power plants) that convert energy from its form as mass to other forms.

The corresponding united theory of information and entropy is not as well developed, for several historical reasons. The contemporary philosophical approach includes the models, where entropy is one kind of information, and there are other kinds as well. Like energy, information can reside in one place or another, it can be transmitted through space, and it can be stored for later use.

Second Law states that entropy never decreases as time goes on – it generally increases and may only in limiting cases remain constant. In the present case, the new approach is to start with information and work from there to entropy, and the new organizing principle is the united theory of information. A key, for example, carries information about the lock that it fits, whereas this text is information because it corresponds to presumable patterns in the brains of the author and the reader. More specifically, information is defined as the correlated entropy between two ensembles, and the ambiguous concept of entropy represents a fundamental link between thermodynamics and information theory. This link between matter and information is most evidently manifested by the molecular constitution of the genetic code, and represents the core of modern life science [12]. Genetic information, in the form of nucleic acids, is propagated by a thermodynamic mechanism that may be described as template replication of aperiodic polymers, and this surprisingly simple concept combines the replication and variability that underlies Darwinian evolution [13]. In principle therefore, the origin of life may be explained by the spontaneous rise of template-replicating polymers. But despite significant advances in the field of autocatalytic and self-replicating chemistry, selforganization of template-replicating polymers from individual monomer, independent of complex catalysts, has not been demonstrated. This inability to physically demonstrate spontaneous rise of genetic information represents a definitive missing link between thermodynamics, information theory, and life science, and has been embraced as a key argument by those who oppose a scientific explanation for life.

Modern Information Science (MIS) main channels were created by N. Winner and C Shannon [14], when they describe the negative entropy as main source of unquantitative information.

One of the very practical and well developing ways of MIS is molecular modeling, also known as molecular mechanics, which is a method to calculate the structure and energy of molecules based on nuclear motions. Electrons are not considered explicitly, but rather it is assumed that they will find their optimum distribution once the positions of the nuclei are known. Molecular mechanics allows computational modeling of the positions and trajectories of the nuclei of individual atoms without an undue computational load. Current packages available on personal computers can readily do energy minimizations on systems with thousands of atoms, while supercomputers can handle systems with hundreds of thousands of atoms or more. More complex analyses, particularly analyses that involve searching through large configuration spaces, can limit the size of system that can be effectively handled. As will be discussed later the need to search through large configuration spaces (as when determining the native folded structure of an arbitrary protein) can be avoided by the use of relatively rigid structures (which differ from relatively floppy proteins and have few possible configurations). The modeling of machine components in vacuum reduces the need to model solvation effects, which can also involve significant computational effort. In molecular mechanics the individual nuclei are usually treated as point masses. While quantum mechanics dictates that there must be a certain degree of positional uncertainty associated with each nucleus, this positional uncertainty is normally significantly smaller than the typical internuclear distance. While the nuclei can reasonably be approximated as point masses, the electron cloud must be dealt with in quantum mechanical terms. However, if we are content to know only the positions of the nuclei and are willing to forego a detailed understanding of the electronic structure, then we can effectively eliminate the quantum mechanics. For example, the H_2 molecule involves two nuclei. While it would be possible to solve Schrodinger's equation to determine the wave function for the electrons, if we are content simply to know the potential energy contributed by the electrons (and do not enquire about the electron distribution) then we need only know the electronic energy as a function of the distance between the nuclei. That is, in many systems the only significant impact that the electrons have on nuclear position is to make a contribution to the potential energy E of the system. In the case of H_2, E is a simple function of the internuclear distance r. The function E(r) summarizes and replaces the more complex and more difficult to determine wave function for the electrons, as well as taking into account the inter-nuclear repulsion and the interactions between the electrons and the nuclei. The two hydrogen nuclei will adopt a position that minimizes E(r). As r becomes larger, the potential energy of the system increases and the nuclei experience a restoring force that returns them to their original distance. Similarly, as r becomes smaller and the two nuclei are pushed closer together, we also find that a restoring force pushes them farther apart, again restoring them to an equilibrium distance. More generally, if we know the positions r_1, r_2, ... r_N of N nuclei, then $E(r_1, r_2, ... r_N)$ gives the potential energy of the system. Knowing the potential energy as a function of the nuclear positions, we can readily determine the forces acting on the individual nuclei and therefore can compute the evolution of their position over time. The function E is a newtonian potential energy function (not quantum mechanical), despite the fact that the particular value of E at a particular point could be computed from Schrodinger's equation. That is, the potential energy E is a newtonian concept, but the particular values of E at particular points are determined by Schrodinger's equation. This assumption is based on the Born-Oppenheimer approximation of the Schrödinger equation. The Born-Oppenheimer approximation states that nuclei are much heavier and move much more slowly than electrons. Thus, nuclear motions, vibrations and rotations can be studied separately from electrons; the electrons are assumed to move fast enough to adjust to any movement of the nuclei.



In a very crude sense molecular modeling treats a molecule as a collection of weights connected with springs, where the weights represent the nuclei and the springs represent the bonds.

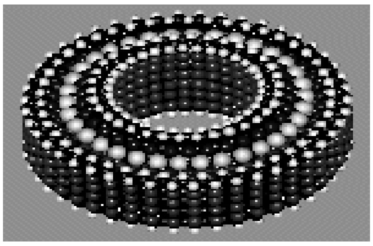
A *force field* is used to calculate the energy and geometry of a molecule. It is a collection of atom types (to define the atoms in a molecule), parameters (for bond lengths, bond angles, etc.) and equations (to calculate the energy of a molecule). In a force field a given element may have several atom types. For example, ethylbenzene contains both *sp*^{3}-hybridized carbons and aromatic carbons. *sp*^{3}-Hybridized carbons have a tetrahedral bonding geometry, while aromatic carbons have a trigonal bonding geometry. The C-C bond in the ethyl group differs from a C-C bond in the phenyl ring, and the C-C bond between the phenyl ring and the ethyl group differs from all other C-C bonds in ethylbenzene. The force field contains parameters for these different types of bonds. Some of these parameters are given below. The total energy of a molecule is divided into several parts called force potentials, or potential energy equations. Force potentials are calculated independently, and summed to give the total energy of the molecule. Examples of force potentials are the equations for the energies associated with bond stretching, bond bending, torsional strain and van der Waals interactions. These equations define the potential energy surface of a molecule.

$$\mathbf{E_{TOTAL} = E_{STRETCH} + E_{BEND} + E_{S\text{-}B} + E_{TORSION} + E_{vdW} + E_{DP\text{-}DP}}$$

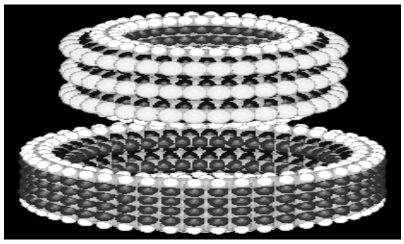
Below are examples of some of the force potentials, and parameters one may find in a force field [15,16].

Computational experiments also provide more information. For example, molecular dynamics can literally provide information about the position of each individual atom over time, information which would usually be inaccessible in a physical experiment. Of course, the major advantage of computational experiments over physical experiments in the current context is the simple fact that physical experiments aren't possible for molecular machines that we can't make with today's technology. By using computational models derived from the wealth of experimental data that is available today, we can (within certain accuracy bounds) describe the behavior of proposed systems that we plan to build in the future. If we deliberately design systems that are sufficiently robust that we are confident they will work regardless of the small errors that must be incurred in the modeling process, we can design systems today that we will not be able to build for some years, and yet still have reasonable confidence that they will work. By fully utilizing the experience that has been developed in the rapid design and development of complex systems we can dramatically reduce the development time for molecular manufacturing systems. It is possible to debate how long it will be before we achieve a robust molecular manufacturing capability. However, it is very clear that we'll get there sooner if we develop and make intelligent use of molecular design tools and computational models. These will let us design and check the blueprints for the new molecular manufacturing technologies that we now see on the horizon, and will let us chart a more rapid and more certain path to their development.

Each of the steps of pulling a rod up against another and then releasing it is a mechanically reversible operation. As each spring is stretched and un-stretched, work is done and then recovered. Assuming that the motions are slow and smooth, the whole process is thermodynamically reversible. Charles Bennett and Ed Fredkin (of MIT) along with Rolf Landauer have described the thermodynamics of computation and they conclude that this kind of combinatorial logic can in principle be thermodynamically reversible [17]. In the limit of slow motion, this system matches that ideal. The main loss results from one knob losing vibrational freedom as it is pushed against another knob. That is like compressing a gas molecule in a cylinder. If you do it slowly enough, the process is isothermal and reversible because the temperature of the gas is the same after it has expanded as before it was compressed and the force applied on the way in is the same as what you get back on the way out. If instead the compression is done fast, the gas heats as it is compressed and then cools as it expands. In this case you get less work out as it expands then you put in to compress the gas so that you have a thermodynamic irreversibility.

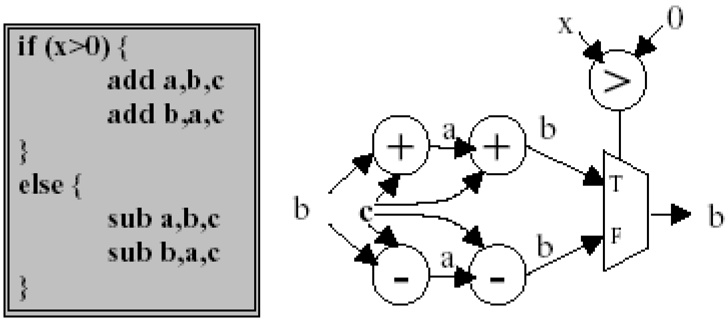


A molecular bearing



The bearing taken part

Graph representation of molecular structures is widely used in computational chemistry and theoretical chemical researches [18]. Molecular structures are represented by graphs where vertices correspond to atoms, and edges to chemical bonds. This kind of a graph, called now a molecular graph, is the object of study in the theory of ordinary graphs. However ordinary graphs do not adequately describe chemical compounds of nonclassical structure. A substantial drawback of the structure theory is the lack of a convenient representation for molecules with polycentric bonds. Most often polycentric bonds are encountered in organometallic (sandwich type) compounds, polycyclic conjugated molecules, benzenoid systems in particular, etc.



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In summary, it is quite possible to adequately model the behavior of molecular machines that satisfy two constraints: (1) they are built from parts that are sufficiently stable that small errors in the empirical force fields do not raise significant questions about the shape or stability of the parts, and (2) the synthesis of the parts is done by using positionally controlled reactions, where the actual chemical reactions involve a relatively small number of atoms whose behavior can be adequately modeled with higher order ab initio methods.

Clearly, not all molecular machines satisfy these constraints [19]. The range of molecular machines which do satisfy these constraints sufficiently large to justify the effort of designing and modeling them. And, in particular, we can satisfactorily model Drexler's assembler within these constraints. The fundamental purpose of an assembler is to position atoms [20]. To this end, it is imperative that we have models that let us determine atomic positions, and this is precisely what molecular mechanics provides. Robotic arms or other positioning devices are basically mechanical in nature, and will allow us to position molecular parts during the assembly process. Molecular mechanics provides us with an excellent tool for modeling the behavior of such devices [21,22]. The second fundamental requirement is the ability to make and break bonds at specific sites. While molecular mechanics provides an excellent tool for telling us where the tip of the assembler arm is located, current force fields are not adequate to model the specific chemical reactions that must then take place at the tip/work-piece interface involved in building an atomically precise part. For this, higher order ab initio calculations are sufficient. The glaring omission in this discussion is the modeling of the kind of electronic behavior that occurs in switching devices. Clearly, it is possible to model electronic behavior with some degree of accuracy, and equally clearly molecular machines that are basically electronic in nature will be extremely useful. It will therefore be desirable to extend the range of computational models discussed here to include such devices. For the moment, however, the relatively modest inclusion of electrostatic motors as a power source is probably sufficient to provide us with adequate "design space" to design and model an assembler.

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