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A conceptual model of microtubules as a macrobiological molecule and Quantum Consciousness

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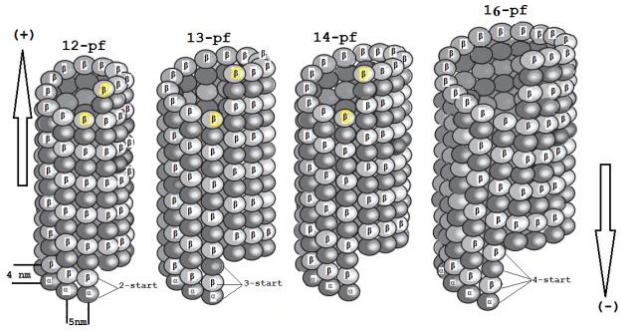
ABSTRACT

Alzheimer's is a kind of psychosis that causes problem with brain, thought and memories. Ii is usually reveals slow and slow to get worse with daily activities. In this work the relationships between Alzheimer's desease, consciousness and brain's memories with microtubule as macro- molecules have been shown and expanded with a wide discussion. In the primary epistemologically levels, those are a mathematical equations related to the Orch-OR theory, which might be explain the root of the Orch OR theory distances for explaining the full function of the brain. In the second part, it has been referred to one part of the equation it computes a portion of consciousness and exhibiting the mechanism of consciousness's effect to changing the physiological phenomenon of microtubules as macromolecules.

Keywords: Psychology, *Physiology, Orch OR theories, microtubules, consciousness, evolution.*

1. INTRODUCTION

Microtubule (MTs) is included of protein filament with a dynamical cytoskeletal structure consist of morphological changing. Microtubules are consist of two tubular polymers and its diameters of each are about 25 nm in which the heterodimer is assembled head to tail in the polar fashions (scheme 1). MTs have a multiple structure with unique function in the cellular mechanism for a peculiar biophysical setting in the internal surrounding of the cells. These "structures" from that those are combination that called alpha and beta-tubulins which are proteins and occurs in solution as a dimer for two similar subunits with their assemblies which are in a part determined through the consciousness of two tubulins in the cytoplasm (scheme.1). recently, two scientists, 1-Roger Penrose, and 2-Stuart Hameroff, approval that conscious nesses have a largely non-algorithmic natures and relies on quantum mechanics [1,2]. The current leading candidates for a computer-like neural correlate of consciousness involve neuronal circuits oscillating synchronously in the thalamus and cerebral cortexes. Higher-frequencies oscillations have been suggested for mediating the temporal binding of consciousness experience [4-6]. As Hameroff's theories conventional explanations portray consciousness as the emergent properties of classical computer-likes activities in the brain's neural networks. Those have been proposed which in the human's brains there are the superposed state of 120, quantum dot register which are also the number of superposed tubulins- digits in any brain [7, 8]. It has been postulated which elementariness particles are also possessed through the consciousness. In addition, the consciousness's brain is lost in in-animate matter because of two non-alignment of the consciousness vector in the elementary particles constituting the inanimate matter. Those digits in the brains undergo the orchestrated objective reduction which leads to the conscious events [9]. These might be explained through quantum computational points of view [10, 11]. Based on proponents of this deep ecologies, there are important-enchantment of the world and honors and embraces every animate and inanimate elements on the earth. These consciousness vectors of the in-animates matter will increase for become conscious under ideal conditions. Similarly, consciousness vectors of the living organism will be increase resulting in a higher state of consciousness for the living organisms [12-15].



Scheme 1: The schematic images of various microtubules including "12-16" proto-filaments

The question is arisen why during reduction superposition becomes the global mode but in the opposite direction the state of the universes is not converted to the superposition of those states.

According to the previous article [16, 17], the process conversion of consciousness for realizing is the nature of the brain. It is because of space and time and the state away from each other**.** So after each change in consciousness happen on the realities of changes and any changing in the consciousness equals are the reality of changes. In the meaning theory of Hameroff's interiors for living cells are functionally organized through webs of protein polymers the cytoskeleton. Major component of the cytoskeleton are microtubules, self-assembling hollow crystalline cylinders whose walls are hexagonal lattices of subunit proteins known as tubulins. Microtubules are essential for the varieties of biological functions including cell movements, cell divisions (mitosis's cell)

and establishment and maintenance of cell forming and functions [6-14].

In neurons, microtubules self-assembling for extending axons and dendrites to form synaptic connections; microtubules then help maintain and regulate synaptic strengths responsible for learning and cognitive functions. While microtubule has traditionally been considered as purely structural component, recent evidences have demonstrated mechanical signaling and communication function. Microtubules interact with those membrane structures and activate through linking protein and `second-messenger' chemical signal. The overall structure of the tubulin-statement's complexes has been suggested through scanning transmission electron microscopy combined with digital image processing [17, 18]. Many research and works have been accomplished for characterizing structurally with the three major forms of 1-microtubules, 2-heterodimers, and 3-curved Proto-filaments. Gigant et al. [19] reported the 4.1-A˚ X-ray structures of the complexes of GDP-tubulins with the *"Escherichia coli*" explicit stathmin-like domains for RB3 (RB3-SLD), the stathmin families proteins. These shape defines the 3D structures of the complexes, the arrangement of tubulins within these complexes, are shown that RB3 contacts tubulin through a 90-residue α- helix.

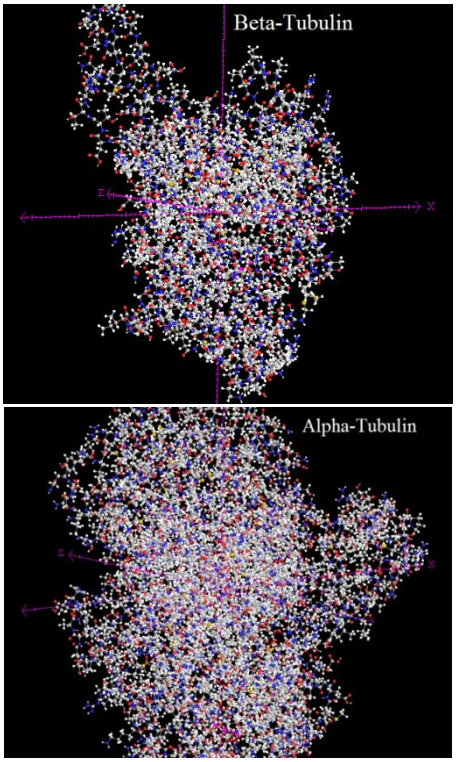


Figure 1: Alpha& beta Tubulin optimized through QM/MM and OPLS charm methods.

2. EXPERIMENTAL SECTION

2.1. Theoretical background. The atomic structures of tubulin proto-filaments are discovered with electron crystallographers of the Zn induced two dimensional sheets [20]. There are binding sites for the guanidine nucleotides on the end region of these domains that contact is made with the next subunit in the proto-filaments. The binding sites for "Taxol" are placed on the second domain of $\alpha\beta$ -tubulin, which also make contact with the core helix, to the opposite sides from nucleotide base Fig.1. Ravelli [21], extracted wonderful information concerning the conformation structures through X-ray crystallography. Each unit has a pair of spherical domains that the largest domains, containing the N-terminal of its polypeptides, have the same folding as a "Rossmann folding" [20, 21].The C-terminals end of each tubulins polypeptides make two long helices which those residues (from C-terminal) might be suitable for isoform recognition by tubulin binding proteins. In a few position the proto-filaments makes a ring through bending at the interface among the monomers. The bending of proto-filaments was first seen via electron microscopies spectrum [22] and has been confirmed in co-crystals of tubulin-sequestering of stathmin protein by Gigant et al [23]. As it has been shown (Fig.1&2) some of the long loops of the globular domain is combined as a complex with lateral contacts among the proto-filam ends in the microtubule. In addition, there are common agreement that the "M-loops" of one proto-filament make contact with the guanidine triphosphate (GTPase) domain and the M-loop make different contacts with the adjacent proto-filament (Fig.1).

The bending will be visible even in the absence of destabilizing agents as the same stathmin or colchicine. Although several stathmin have been introduced, the mechanism by which kind of stathmin affects microtubules dynamics are a title of argument. The core helixes are means of communication from the top to the bottom of the β-subunit through cooperative mechanism. Whole microtubules can twist and bend without coming images of fluorescently labeled microtubules growing [24]. When the microtubule is bended, the individual proto-filaments one by one are bent in several directions. In this investigation, It has been found in vitro that the effects of stathmin might be concluded from abilities for forming the strong bonded and non-bonded interactions through a ternary complexes including two subunits of α and β tubulins, αβ dimer of two tubulins and another stathmin Fig.2. Therefore, there are multiple "bent" states for dimers and proto-filament and there are no curved conformation induced by different agents of disassembles.

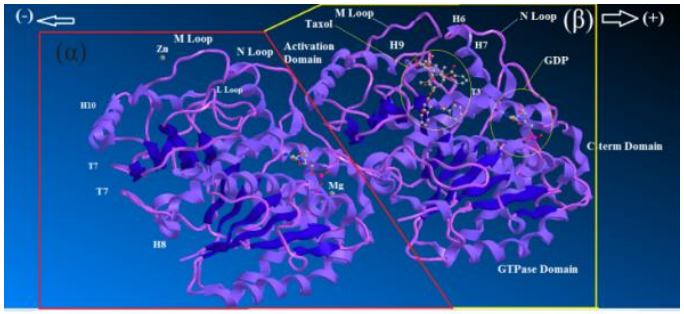


Figure 2: Ribbon diagram of αβ -tubulin heterodimer, the structure solved by electron crystallography using sheets of bovine brain [21].

Several attempts have accomplished for characterizing three main forms of microtubule's structures, in view point of heterodimers, and also curved Proto-filaments. The whole structures of the tubulin-stathmin complexes have been suggested through scanning

transmission of electron microscopies combined with digital imaging [25]. Formation of tubulins-stathmin complexes indicated a new way for stabilizing tubulins in for the crystal. Benoıt Gigant et al. [19, 23] has been reported the 4.1 A˚ X-ray structures of the complexes of GDP-tubulin with the *"Escherichia coli*" explicated stathmin-liked domain of RB3 (RB3-SLD-RB3). These kind shapes define the 3D structure of tubulins within its complex. Which exhibit RB3' contacts through a 90-residue of α- helix. Stathmin interacts with two molecules of both α, β-tubulin to form a tight ternary complex in which one mole of stathmin binds to two moles of tubulin dimers through the SLD. The proto-filaments curvature and disassembling has done via GTP hydrolysis. Tubulins are able for switching between the curved structures with the stathmin-like domain of the RB3.

2.2. Methodology. The first opinions for GTPs were thought that they would be allosteric induce to a straight conformation of tubulins thorough-paced of microtubule assembling. The microtubules-associated protein (MAPs) of the tubulin-GDP proto-filament structures has been indicated different intra- and inter-dimer curvature [20-22]. while the GDPs would induce the curved conformational approving disassembles. The evidence for lading of the propositions is the free GTPs-tubulins dimers. Therefore are curved similarly to the two tubulin rings and are driven into the straight conformational structure via the microtubules. However, these types of allosteric mechanism are challenged through the findings of a curved structure of GTPs-bounding γ-tubulin [23]. So the GTPs γ-phosphate only lowers the unfavorable free energies differences between the curved and the straight forms [24, 25].

It is notable, for discussing of the GTP hydrolysis mechanism for destabilizing the microtubule lattice. To provide some answers to these questions, it can be suggested that GTPs hydrolyses into the lattice, but how these strains affects the strength of lateral bonds to destabilize the microtubule remain unknown. Slushing et al., [26] exhibited a structural study for comparing high-resolution of reconstructions of GMPCPP microtubules and GDP microtubules. This compression is amalgamated by conformational changes in α-tubulin. In contrast, lateral contacts between α & β tubulins were basically unchanged in the different nucleotide states. It shows that GTPs hydrolysis induce the compression at the interface between two dimers, quickly over the exchangeable nucleotide-binding sites.

Based on our previous works [27-48] this work has been simulated (Fig.3&4) with microtubule systems including αβ -tubulins heterodimer and stathmin through QM/MM simulation using Monte Carlo method. Thermodynamic averages for the molecular properties were calculated from Monte Carlo theory. The systems were composed of sixteen sections of stathmin molecules including interaction with tubulins [49]. Obviously, at finite temperature, a cluster has finite vaporization pressures, and particular cluster size is typically unstable to evaporation.

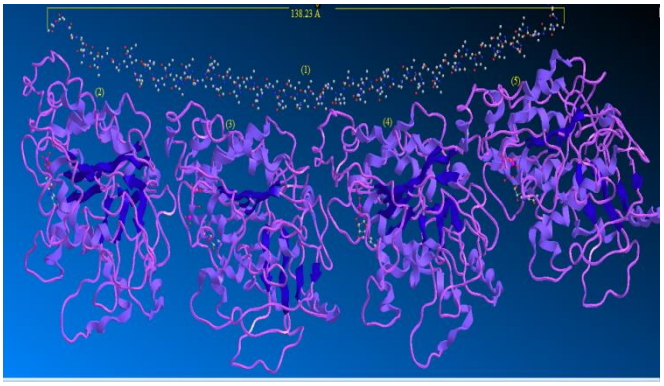


Figure 3: Interaction of stathmin with 4 subunits of tubulin.

2.3. Computational details. Simulation of 16 composed of stathmin molecules were carried out for microtubules. With a mean field was generated through Monte Carlo (MC) method, to obtain agreement with experimental order parameters. In this investigation, differences in force field are accomplished through comparing the calculated energies by using force fields AMBER and OPLS. The pressures were fixed by extended system formalism, the Langevin Piston algorithms, reduces oscillations in the cell membrane and also for configurations of αβ -tubulin heterodimer and stathmin. The temperature was fixed at body temperature (300 K). Inaddition, Hyper-Chem professional release 7.01 is used for these calculations. We applied density functional theory with the van der Waals DFT for modeling the exchange-correlation energies of αβ -tubulin heterodimer. The final parameterizations of stathmin were done using self-consistent field calculation in order for finding the optimal starting geometries, as well as the partial charges. We mainly focused on the results from DFT methods such as m062x, m06-L, and m06 for the αβ -tubulin heterodimer. All optimization of 16 section of stathmin monomer were performed through Gauessian and GAMESS-US packages.

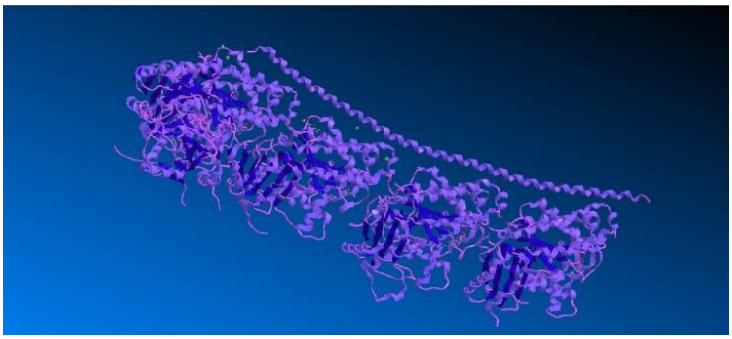
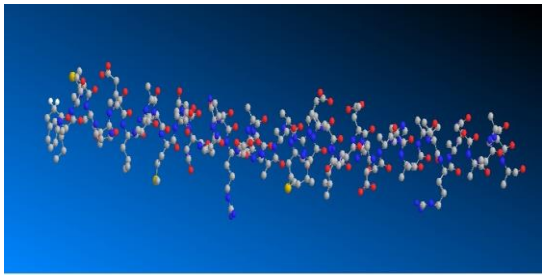


Figure 4: Interaction of stathmin with 4 subunits of tubulin

For non-covalent interactions, the B3LYP method is unable for describing van der Waals microtubules systems by medium-range interactions, therefore the m062x, m06-L and m06-HF are chosen in non-bonded calculations between tubulin heterodimer. The ONIOM methods are also applied with 3 levels of 1-high calculation (H), 2-medium calculation (M), and 3-low calculation. (L) Level performed for calculating the non-bonded interactions between tubulins. The ab-initio and DFT methods were applied for the model system of the ONIOM layers and the semi-empirical methods of AM1, Pm3MM and Pm6 are used for the medium and low layers, the semi-empirical methods have been used in order to treat the non-bonded interactions between two tubulins.

In this work, the arc of stathmin has been divided into two parts Fig. 5. Since the protein busting process is a physical process in which the polypeptide, becomes complex to a certain three-dimensional structure. In most cases, it can be assumed that the natural form of a protein is thermodynamically the most stable for it. Each protein tends to change from a more unstable state to a more stable one.



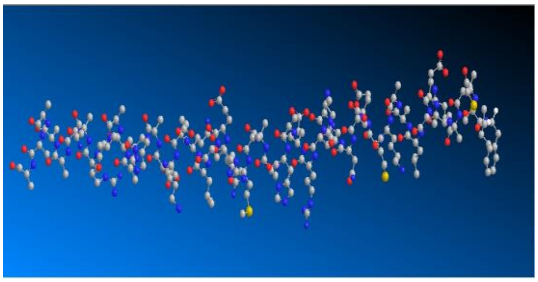
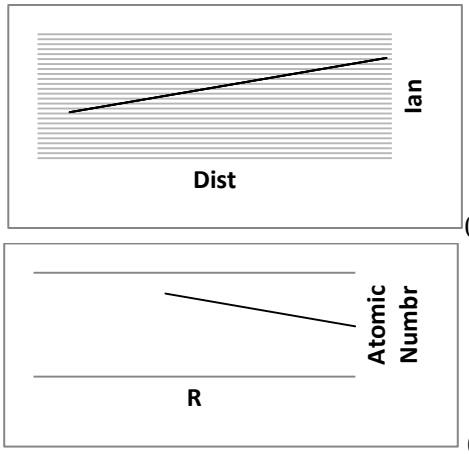


Figure 5: Divided stathmin into two parts A and B

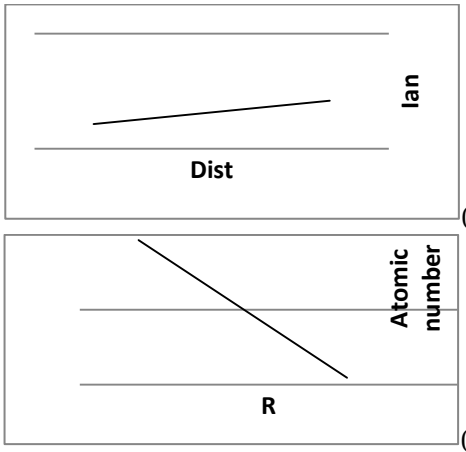
Consequently, it is important to know that proteins have the ultimate form of action, up until eating, which is unique and has the least energy. All the information needed to eat protein in the sequence of its amino acids. Because these unique sequences determine the location of the lateral chains and determine the final shape of the protein.

3. RESULTS SECTION

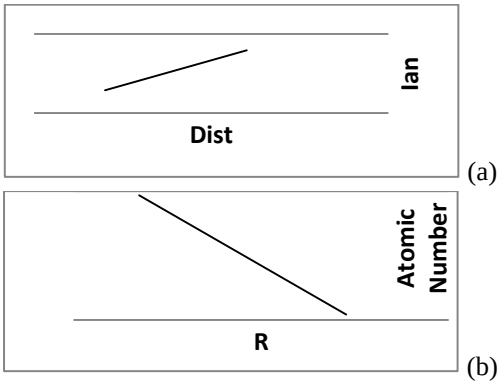
In this work, it has been described a novel method of the step-function models for the microtubules within electron density profile in the composition of the stathmin. In this work, we have focused on the electron density of the systems when each part of two sections in stathmin has interaction one by one with α and β tubulin (Figure 5).



Graf I: Changing chlorine with sulfur in two form a & b



Graf II: Changing bromine with sulfur in two form a&b



Graf III: Changing Iodine with sulfur in two form a&b

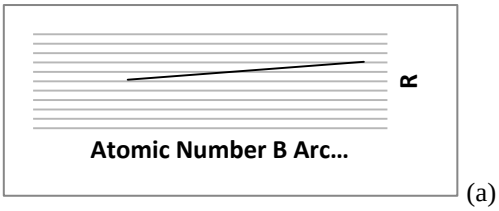
Figure 6: Relation sheep of three halogenated substance in stathmin

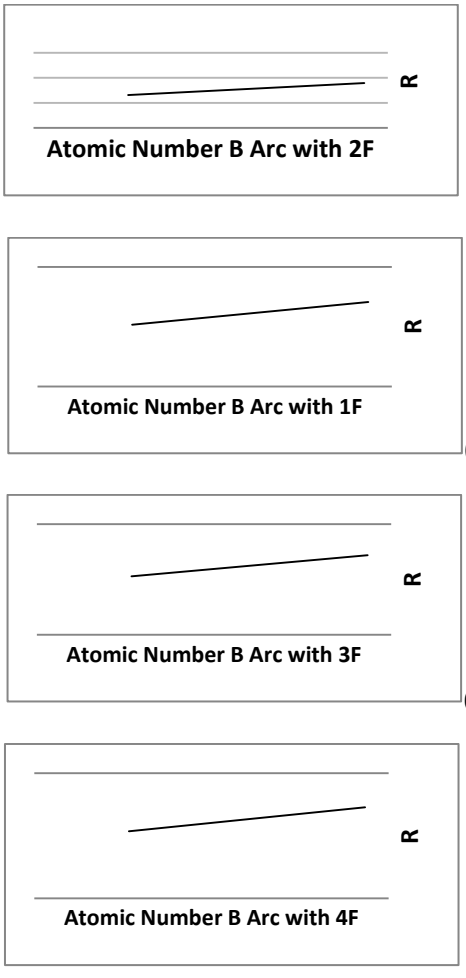
In addition, the effects of atomic changing and atomic Number Factor with R have been considered. The graphs IV represent these changing.

Although the bonded situations and the GTPs hydrolysis essentially is a basic concept for proto-filament curvature and disassembling, the non-bonded interaction explain this processing in other sides. Moreover these kinds of non-bonded interactions provide a dynamic behavior for these approaches.

The proposed quantum superposition/computation phases in neural microtubule correspond to preconscious processing, which continues until the threshold for Penrose's objective reduction is obtained. Objective reduction (OR) discrete event/then occurs, and post-OR tubulin states proceed by classical microtubule automata to regulate synapses and other neural membrane activity.

Graf V: Increase the number of F in B arc.





In this works two major parts have considered for investigating of non-bonded and bonded interaction among 16 parts of stathmin and some halogenated atoms [figs 5-7]. These investigations suggest GTPs hydrolysis introduces strain into the lattice. But how the mechanism strain affect the strength of longitudinal and lateral bond for destabilizing the microtubule remains unknown yet. It seems that changing in the curvature of two αβ-tubulin are basic to microtubule dynamic behavior and the regulatory activities of MAPs (microtubule-associated protein) during microtubule polymerization.

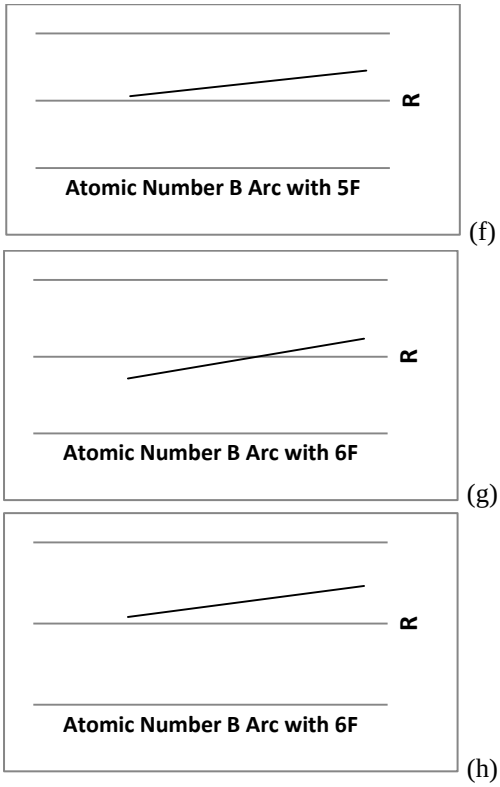


Figure 7: Relation sheep of B and F in various situations (a to h) of stathmin

4. CONCLUSIONS

By this work, it has been illustrated the mechanism of microtubules are depend to two system of tubulins with stathmin curvature. The sections of two parts of stathmin have a specific behavior for a non-bonded interaction between two tubulins and stathmin. This subunit polymerize end to end for any formation of proto-filaments similar to hollow tubes. Its dynamic instability is controlled through numerous molecules. Although the bending occurs even in the absence of destabilizing agents, the core helixes are likely of communication from the top to the bottom of the β-subunit via a cooperative mechanism.

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