

Fig.2 Docking interface of the AxxNIR:Cyt c_{551} complex. (a) The building block of the interface. The amino acid residues at the protein interface and the TICu ligands are represented as sticks. The TICu ligands are colored in blue, the residues involved in the hydrophobic patch in gray, and the residues of the "tower loop" in orange. Inset: the residues around the heme group in Cyt c_{551} . The heme group is shown as spheres. (b) Electrostatic potentials of contact protein surfaces. Twenty-five water molecules at the interface are represented as spheres. Eight water molecules bridging between the partner proteins through hydrogen bonds are colored in cyan and the other waters binding to Sub-I or Cyt c_{551} in red.

mation. Contact between these hydrophobic patches brings the redox centers of heme c and TICu within 10.5 Å, which are close enough to allow for rapid ET^{8,9}. Furthermore, 25 water molecules are located at the docking interface. Eight waters bridging the two proteins through hydrogen bonds stabilize the partner proteins, and the remaining waters also provide stabilization through hydrogen bonds and van der Waals contacts to either Sub-I or Cyt c_{551} (Fig.2). All of the water molecules form a characteristic semi-circle around the hydrophobic patch, and the non-polar core interface is sealed off from the aqueous environment.

Superposition of the structure of Cyt c_{551} -docked Sub-I onto that of undocked Sub-II or Sub-III shows an average root-mean-square deviation (rmsd) of 0.7 Å between the corresponding side chain atoms of all the amino acid residues. The most significant structural changes at the interface occur in residues Met87, Met135, Glu195, and Tyr197 (Fig.3). The side chains of Met135 in Sub-II and Sub-III are directed toward solvent. Moreover, HOH516-B in Sub-II and HOH785-C in Sub-III hydrogen bond to the Ne2 atoms of the corresponding solvent-exposed His139 ligands of the TICu site within the range of a typical NH-O bond distance (ca. 2.8 Å). On the other hand, Cyt c_{551} -docked Sub-I has the Met135 side chain tilted toward the imidazole ring of the His139 ligand (Fig.3). The Sδ atom of Met135 is within 3.2 Å of the Ne2 atom of the His139 ligand, and consequently the His139 ligand is no longer exposed to solvent. This behavior of Met135 induced by Cyt c_{551} docking brings about van der Waals interactions between the side chain of Met135 and the non-polar side chains of Val22 and Val28 at the hydrophobic patch around the heme-edge CBC (distance between Cγ2 of Val22 and Sδ of Met135, 3.9 Å; distance between Cγ1 of Val28 and Sδ of Met135, 4.1 Å). In Sub-I, Met135 is therefore sandwiched between the Val residues and tightly fixed over the imidazole group of the His139 ligand; that is, the water molecule bound to the Ne2 atom of the histidyl imidazole ring is removed by movement of the side chain of Met135 and its sulfur atom is in a van der Waals contact with the Ne2 atom. These findings support the locations of three Met residues in the NMR structure the CuNIR (AfnIR):pseudooazurin (PAz) complex from *Alcaligenes faecalis*¹⁰. In the complex, instead of the two Val residues in the AxxNIR:Cyt c_{551} complex, Met16 and Met84 of PAz closely contact to the Met141 residue corresponding to Met135 in AxxNIR. Therefore, in AfnIR:PAz complex, the Met141 tilts toward the His ligand and fixes it. In general, the redox potential of TICu is considerably changed by perturbations of the solvent-exposed His ligand such as protonation and π - π interactions¹¹. The redox potentials of the TICu site of AxxNIR and the heme c group of Cyt c_{551} have been independently determined to be +241 and +290 mV vs. NHE at pH 6.0, respectively. Accordingly, it is likely that the docking of Cyt c_{551} onto AxxNIR tunes the redox potential of TICu through structural constraint and desolvation of the His139 ligand, allowing a smooth interprotein ET reaction. The similar redox potential tuning has been proposed for the TICu sites of amicyanins (Am's) in the binary methylamine dehydrogen-

ase (MADH):Am complex and the ternary MADH:Am:Cyt c_{551} complex¹².

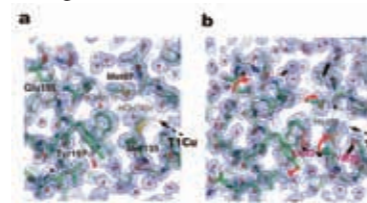
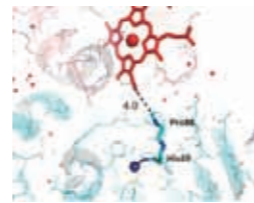


Fig.3 Conformational differences between the Cyt c_{551} -docked and undocked subunits. (a) The Cyt c_{551} -docked Sub-I represented as gray sticks is superposed on the undocked subunit (Sub-III) represented as green sticks. (b) Sub-III depicted as green sticks is superposed on Sub-I depicted as gray sticks. The conformational changes of amino acid side chains in Sub-I having the contact with Cyt c_{551} are indicated with red arrows. Val22 and Val28 close to Met135 in Cyt c_{551} are shown as pink sticks.

Dominant ET pathway

PATHWAY analysis^{13,14} of the AxxNIR:Cyt c_{551} complex was performed to determine the most efficient predicted ET pathway from heme c to TICu. For the purposes of this analysis, the ET donor was defined as the entire heme c group so that the pathway would begin at the most advantageous position on heme c . The predicted pathway through the entry/exit port inside the hydrophobic patches of the interfaces is exhibited in Fig. 4. An electron that leaves iron via the exposed CBC methyl group in the AxxNIR:Cyt c_{551} complex is directly transferred to the Cδ atom of Pro88 of AxxNIR by a through-space jump and then shifts from Pro88 to TICu through the His89 ligand. The ET pathway represents the most favorable route between the redox centers in the core of the hydrophobic interface.

Fig.4 Theoretically dominant ET pathway between heme c and TICu. Interprotein ET pathway in the AxxNIR:Cyt c_{551} complex. The best pathway is shown as a broken-line (through-space process) and sticks (through-bond process). The distance of through-space jump between the CBC methyl group and the Cδ atom of Pro88 is given in angstrom. The heme group (red), the TICu atom (dark blue), and waters (red) are depicted as balls and sticks.



Conclusion

Recognition and interaction between the protein surfaces, as observed in the transient donor-acceptor (Cyt c_{551} -AxxNIR) complex structure occur through sufficient specificity of polar and non-polar interactions, providing a minimal site at the core of the protein-protein interface that ensures the geometry suited for ET reaction. It is particularly important for a deeper understanding of biological ET processes to explore how interface constructions for efficient ET reaction vary with protein-protein shape complementarity, surface charge and polarity, and dynamic fluctuations of the proteins and the organized water molecules at the interface.

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Consistency Management Strategies for Data Replication in Mobile Ad Hoc Networks

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Consistency Management Strategies for Data Replication in Mobile Ad Hoc Networks

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Abstract—In a mobile ad hoc network, data replication drastically improves data availability. However, since mobile hosts' mobility causes frequent network partitioning, consistency management of data operations on replicas becomes a crucial issue. In such an environment, the global consistency of data operations on replicas is not desirable by many applications. Thus, new consistency maintenance based on local conditions such as location and time need to be investigated. This paper attempts to classify different consistency levels according to requirements from applications and provides protocols to realize them. We report simulation results to investigate the characteristics of these consistency protocols in a mobile ad hoc network.

Index Terms—Mobile ad hoc networks, consistency management, data replication, mobile computing.

1 INTRODUCTION

In mobile ad hoc network (MANET) [14], as mobile hosts move freely, disconnections often occur. This causes data in two separated networks to become inaccessible to each other. Preventing the deterioration of data availability at the point of network partitioning is a very significant issue in MANETs [9], [15]. To improve data availability, data replication is the most promising solution [4], [8]. Based on this idea, we have designed effective data replication techniques in MANETs in our previous papers [9], [10], [12]. In [10] and [12], we assume that replicas of a data item become invalid after the host holding the original updates it and the consistency of data operations on replicas is kept in the entire network. However, since network partitioning frequently occurs in a MANET, this strong consistency management scheme heavily deteriorates the data availability. Moreover, many applications in MANETs do not require such a strong consistency. For instance, consider a situation where members of a rescue service that constructs a MANET in the disaster area are divided into several groups each of which is responsible of a certain region and the members in each group share various kinds of information such as that on the extent of damages. In this situation, the consistency of data operations to data items that are used locally in each group must be strictly kept in the same group and is not required to be maintained strictly in different groups.

In this paper, we discuss different consistency conditions of data operations on replicas in MANETs. First, we classify consistency levels according to application requirements.

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Consistency Management Strategies for Data Replication in Mobile Ad Hoc Networks

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Introduction

In a mobile ad hoc network (MANET) which is constructed by only mobile hosts[1], due to the movement of mobile hosts, disconnections of radio links frequently occur. This causes data in two separated networks to become inaccessible to each other. Preventing the deterioration of data availability at the point of network partitioning is a very significant issue in MANETs. To improve data availability, data replication is the most promising solution[2]. However, consistency management of data operations on replicas in partitioned networks becomes a crucial issue. In such an environment, the global consistency of data operations on replicas is not desirable by many applications. Thus, new consistency maintenance based on local conditions such as location and time need to be investigated. This paper attempts to classify different consistency levels according to requirements from applications and provides protocols to achieve them.

Classification of Consistency Levels

Since there are various applications in MANETs such as information sharing in a rescue service and distributed data processing in sensor networks, there cannot be one universal optimal strategy for consistency management. Thus, in this section, we propose four different primitive consistency levels, GC, LC, TC, and PC. Here, which consistency level an application requires is determined based on for what the data obtained by read operations are used in the application and for whom (individual, group, or everyone) the data are useful.

Global Consistency (GC): The consistency of data operations on replicas is required in the entire network. Formally, GC requires that every read operation issued by any mobile host necessarily reads a replica of the latest version in the entire network, i.e., a replica which was written by the latest write operation issued in the entire network. Providing such a strong consistency is generally hard to achieve in MANETs.

Local Consistency (LC): The consistency of data operations on replicas is required only in each region of interest. Thus, this consistency level weakens the strictness of consistency from the spatial perspective. Formally, LC requires that in each region, every read operation issued by any mobile host in the region necessarily reads a replica of the latest version in the region, i.e., a replica which was written by the latest write operation issued in the region.

Time-based Consistency (TC): In TC, replicas are valid even if their versions are different but have not passed a predetermined time (validity period T) since they have been updated

last. This consistency level weakens the strictness of consistency from the temporal perspective. Specifically, when the version of a replica of data item D_j is V_j , i.e., the latest write operation on the replica was performed at time V_j , a read operation on the replica succeeds if the read operation is issued at time A_j on condition that $V_j + T > A_j$.

Peer-based Consistency (PC): The consistency of data operations is required only in each mobile host. Thus, this consistency level further weakens the strictness of consistency than LC and is the weakest from the spatial perspective. Formally, PC requires that at each host, every read operation issued by the host necessarily reads its own replica to which the latest write operation was performed by itself.

Consistency Management Protocols

We describe protocols to realize the four consistency levels given above. Basically, we assume that the area in which mobile hosts can move around is divided into several regions and the consistency of data operations on replicas is managed based on the regions. There exist two kinds of mobile hosts; proxies and peers. A proxy is a specially designated peer who manages other peers in a specific region in the MANET.

Global Consistency (GC): To achieve GC, we hierarchically adopt dynamic quorum systems[3] inside each region and inter regions (i.e., the entire network). In a quorum system, read and write operations are performed on only replicas held by mobile hosts that form read and write quorums, respectively, where every pair of read and write quorums have an intersection. Since there is an intersection between write and read quorums, at least one mobile host in a read quorum holds a replica of the latest version and thus the consistency of data operations can be kept by reading the latest version.

The quorum size for a write operation (to any data item), $|QW|$, and that for a read operation, $|QR|$, in the entire network are determined where the condition, $|QW| + |QR| > l$, is satisfied. Here, l is the total number of regions (proxies) in the entire network. Moreover, in each region R_i ($i=1, \dots, l$), the quorum size for a write operation on data item D_j , $|QLW_{ij}|$, and that for a read operation, $|QLR_{ij}|$, are determined where the condition, $|QLW_{ij}| + |QLR_{ij}| > P_{ij}$, is satisfied. Here, P_{ij} is the total number of peers that hold D_j in the region.

When a peer in a certain region issues a read (write) request, it first sends the request message to the proxy in the region. Then, the proxy tries to construct a read (write) quorum in the region and also ask proxies in other regions to construct a quorum in their regions (Fig.1). If more than $|QLW_{ij}|$ ($|QLR_{ij}|$) proxies successfully construct a quorum, the request succeeds

and the operation is performed.

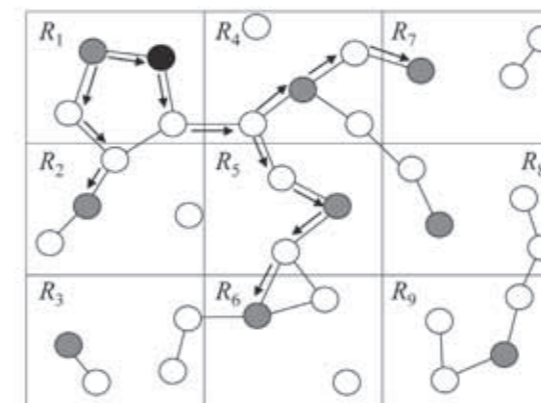


Fig.1 Example of executing GC. A request issued by a peer (back circle) in R_1 is handled by the proxy (gray circle) in R_1 , where the proxy contacts five proxies (gray circles) in $R_2, R_3, R_4, R_5,$ and R_6 .

Local Consistency (LC): The protocol to achieve LC is almost identical to that inside region in the GC protocol. Specifically, the request-issuing peer tries to construct a quorum in its region. If it succeeds, the operation is performed.

Time-based Consistency (TC): The protocol to achieve TC does not need to control write operations, i.e., write operations can be performed on any replicas. On the other hand, read operations need to find a valid replica. If the peer that issued a read operation request holds a valid replica, it can perform the operation locally. Otherwise, it first tries to find a valid replica in its region by flooding the request message in the region. If it still fails, it tries to find a valid replica in the entire network.

Peer-based Consistency (PC): Each peer can perform read and write operations anytime on its own replica and no special mechanism is needed.

Performance Evaluation

In this section, we show simulation results to investigate the characteristics of the proposed consistency levels and protocols. 240 mobile hosts (M_1, \dots, M_{240}) exist in an area of $X \times Y$ [m²] which consists of 12 regions (R_1, \dots, R_{12}) of $X/3 \times X/3$. Here, ratio $X:Y$ is kept to 3:4. In our experiments, X is changed as a variable parameter in the range from 300 [m] to 600 [m]. M_i ($i=1, \dots, 12$) is the proxy of region R_i . The number of data items in the entire network is 500.

Fig. 2(a) and Fig. 2(b) respectively show the success ratio of write operations and that of read operations for the proposed four protocols. From the results, the success ratios of both read and write operations in GC and LC get lower as the area size gets larger. This is because the connectivity among mobile hosts becomes lower, thus, the necessary number of replicas to construct a quorum cannot be found with high probability. We can see an interesting fact that when the area size is larger than 450, the success ratio in GC suddenly gets lower but in LC remains high. This fact shows that even when the connectivity among mobile hosts is still high in each region, the connectivity among proxies becomes low.

The success ratio of write operations in TC and those of write and read operations in PC are always 1 because every operation can be executed locally. The success ratio of read operations in TC gets lower as the area size gets larger. This is because when the connectivity is low, mobile hosts cannot access valid replicas held by connected mobile hosts with high probability. Comparing LC and TC, TC always gives a lower success ratio, although TC weakens consistency from the temporal perspective.

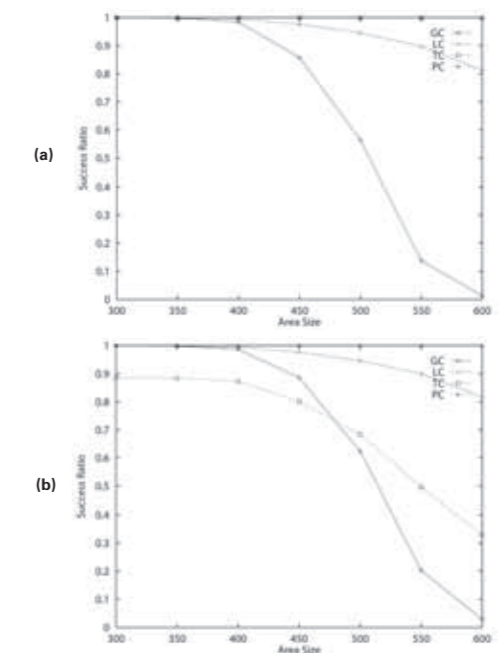


Fig.2 Simulation results varying the area size: (a) request success ratio of write operations and (b) request success ratio of read operations.

Conclusions

In this paper, we have classified consistency levels in MANETs according to applications' demand, and then, have designed protocols to achieve them. We have conducted simulations to investigate the behaviors and features of our proposed protocols. From these results, it is shown that the performance of the proposed protocols much differs with each other and that we should choose LC rather than GC in terms of success ratio if applications do not require the strict consistency in the entire network.

As part of future work, we plan to consider replication strategies suitable for each consistency level.

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