Correlation between NaCl concentration and solvent water dynamicalbehavior

: An observation by data mining method

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Salt water is one of the most familiar solutions, and many researchers are interested in its feature. The solution molecules behavior is observed by using computer simulation to research the feature (ex. ions and water molecules correlation, structure, behavior and so on). Recently, the simulation can calculate big scale and long time by development of computational science and technology, and the simulation date became huge size. In these days, date mining is attracted attention as the method analyses huge date efficiently. The purpose of my work was to analyze the behavior of the salt water molecular by using molecular dynamics simulation and date mining. For the purpose of this paper is to simulation five kinds of salt water model dynamics and to analyze water molecules trajectory of the solutions by using date mining. As a result, water molecular show particular behavior. It is concluded from the result that ions make network and water clusters.

1. Introduction

The existence of water is one of the essential factors for our life. Until today, many researchers have been interested in the water behavior from the viewpoint of not only physical property, chemical property, but also life science field such like taste of water, human health. In experimental study, water behavior can be analyzed in nano scale observation. However, it is difficult to catch up all of dynamics and behavior of each water molecules to characterizing

Table 1 Water Models

concentration	*0.43%*	*1.64%*	*4.74%*	*6.18%*	*32.30%*	*40.20%*
residue	4505	4505	4505	4505	4505	4505
Na+	6	23	68	90	577	774
Cl-	6	23	68	90	577	774
water	4493	4459	4369	4325	3351	2957

the water structure in relation to physical, chemical property and life science interested. Recently, the development of computational science and technology provide us a sufficient environment for reproduce the water behavior as the huge system including more than 10,000 water molecules by using molecular dynamics (MD) simulation.

In this study, we investigate the dynamical structure of water molecules by using data-mining techniques for the huge amount of trajectory data of water molecules generated by MD simulation. Classification and comparing the water dynamics of system including ions (Na+, Cl-) and pure water system, we suggest a new indicator, which can represent the special feature of water behavior, to support the analyzing of relation between dynamical structure of solvent and essential property in life science field (i.e. taste sense).

2. Experiment

In this study, we perform classical MD simulation for 5 kinds of solvent models with different NaCl concentrations (TIP3P model : 0%, 0.43%, 1.64%, 4.71%, 32.3 and 40.2%) shown in Table 1. In each simulation, both TIP3P and TIP4PEW water models are adopted to neglect the water model dependency TIP3P models. All MD simulations are performed under the room temperature (300K) constant volume condition with periodic boundary by Amber 10 program package with force field 03. The cutoff radius is 12 Å for long range interactions. Total simulation time of all models is 10 ns (1 MD step = 20 fs). The trajectory data is stored in each 20fs.

In order to quantify the behavior of (hydration) water molecule in a moderate condition (300 K, 1 atom), we applied data mining techniques to the coordinates of water molecules which were stored by the molecular dynamics (MD) simulation.

The data mining process is consists from four parts.

1) Carry out MD simulations of the motion of water molecules in interaction with proteins: the moving of each water molecule is measured in a time interval Δt.

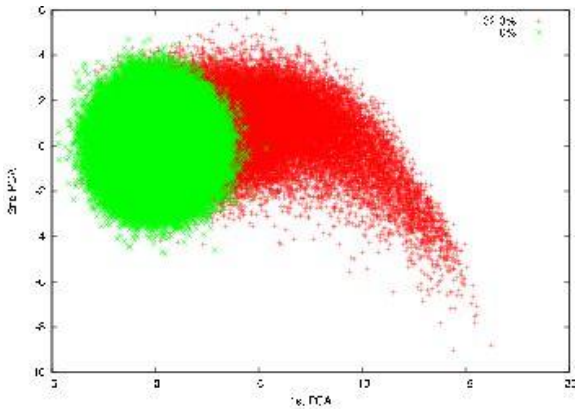


Figure 1 Analysis Result Pure and 32.3% NaCl Water in Pure and 32.3% NaCl % Water

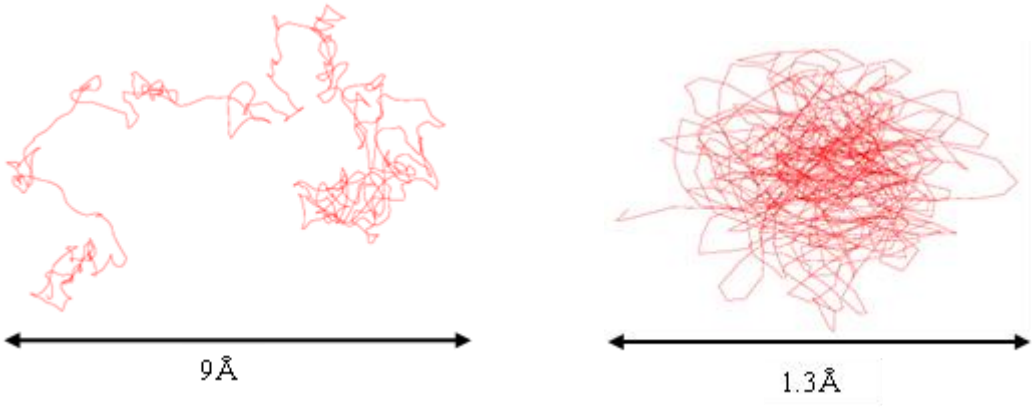
2). Transform the moving data into a new feature space that represents moving behavior of the water molecules.

3). Develop an appropriate clustering method to model the structure of water in protein solution as clusters by water molecule moving behavior. These clusters in a given time interval Δt are called static structure.

4). Investigate the dynamics of hydration water and the dynamic structure of water surrounding proteins from the stream of static structures created in consecutive time intervals by steps 1-3.

3. Result and Discussion

At first, we confirm the energy stability of each simulation. Because of converge time of total energy is similar in each models, equilibration this is not affected by exist one of ions. So, analyzing date can collect from same term interval. We analyzed stability terms by using date mining.



Quintessential Water Structure **particular Water Structure**

Figure 2 Quintessential and Particular Water Behavior in 32.3% NaCl solution in 20 ps.

By using the trajectory datasets in equilibrium period. PCA projection is carried out for a multipole expansion water dynamics defined in section 2. 1st and 2nd principle components are mapping in the one plane. Compare the water dynamics of each molecules in PCA space shown Figure 1, some waer molecules in NaCl solution are mapped in outside from the normalized mapping of pure ware system perturbation effect of such kinds of new water behavior is the evidence of Na and Cl ions.

These modes show one distinctions. In high concentration (32.3% saturated saline), discriminative particular mode is increased. Figure 2 shows one of trajectories in 32.3% NaCl solvation. The trajectory which is shown by Figure x is

From this results, water molecules behaviors in NaCl solvation have particular mode.

4. Conclusions

In this study, we suggest a new analytical approach to solve the taste sense by MD simulation and date mining. From the result, we found that the variety is decreased, and particular modes with cooperative motion are increased in high concentration 32.3% NaCl solvation) and show the particular trajectory which don't move other coordinate. This result indicates Na and Cl ions make network and water clusters like hydrate.

In future works, we will research correlation ions' network and water molecular clusters. Moreover, we will also research NaCl hydrate by using simulation and datamining..