Distribution of Water Molecules in a Triboelectric Charging System

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Contents

1 Background

Triboelectric charging is a well-known phenomenon of physics which occurs when two different materials were brought into contact and then separated. However the understandings on this phenomenon is quite limited. There is neither a good way to predict the direction of this kind of charging nor a method to explain why the material got charged after contacting or rubbing with another material.

In previous laboratory works, researchers found that the result of their experiment varies when there is some moisture on the surface of the material. So the behavior of water in such system becomes an interesting topic so as to the role that water molecule plays in the charging process.

2 Aim of the project and approach

2.1 Aim

To analyze the distribution of water molecules in a triboelectirc system using datas provided by a molecular dynamic simulation.

2.2 Approach

The distribution of water molecules will be analyzed using the density of water calculated in each unit volume.

ggplot2 package will be used for the visualization of the results.

R packages will be used to do the calculations and process the data files.

3 Data source and structure

3.1 Source

The data will be aquired from a MD simulation performed on a triboelectric charging system carried out using SEISTA software package.

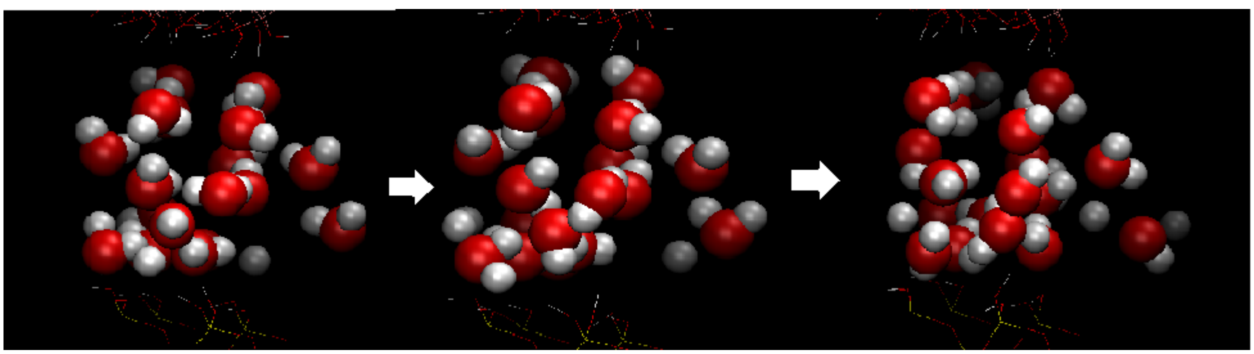


Figure 1: 'Some images from the simulation'

4 Target Data Structure

The coordinate data extracted from the raw data file is stored in a data frame. The data frame has four columns which contains the name of the atom, x, y and z. Since I'm interested in the water molecules, only the data for water molecules were kept in my data frame and the data for other materials involved in the model were not recorded.

My target coordinate data structure is a list of data frames. The xyz values for each H and O atoms at each time step consists each frame and the frames are stored in the list by the order of time.

The target density data structure is a data frame consist of the density value for each segment of z at each time.

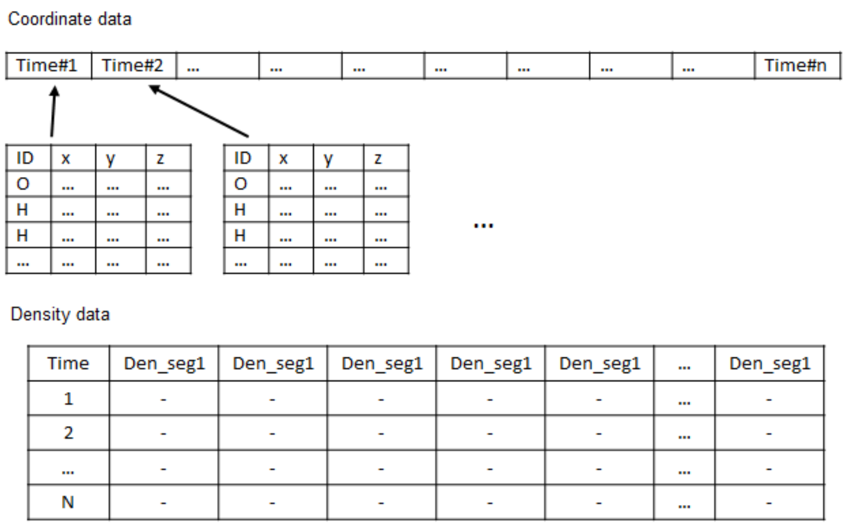


Figure 2: “Data structure”

5 Data cleanning & creation of databook

The position of an atom is recorded in cartesian coordinate. The unit for x, y and z values is angstrom.

5.1 Get data from data files

```
setwd(dir = "../../data/")
file_list<-list.files(pattern=".ANI")
#original data files
file_list
```

```
##  [1] "01.ANI" "02.ANI" "03.ANI" "04.ANI" "05.ANI" "06.ANI" "07.ANI"
##  [8] "08.ANI" "09.ANI" "10.ANI" "11.ANI" "12.ANI" "13.ANI" "14.ANI"
## [15] "15.ANI" "16.ANI" "17.ANI" "18.ANI" "19.ANI" "20.ANI"
```

```
#construct raw dataframe
temp<-data.frame()
data_book<-NULL
for (i in 1:length(file_list)) {
  temp<-read.table(file_list[i],fill = T)
  data_book<-rbind(data_book,temp)
}
colnames(data_book)<-c("ID","x","y","z")
rm(temp,file_list)
data_book[c(1:10,316:326),]
```

```
##       ID        x         y        z
## 1    322       NA        NA       NA
## 2     Al 0.062262 -0.061474 27.99369
## 3     Al 0.023524 -0.062809 23.60832
## 4     Al 2.479899 -1.541318 30.45027
```

```
## 5    Al 2.453591 -1.478855 21.63416
## 6    Al 2.430596 -1.426610 27.98369
## 7    Al 2.410617 -1.432265 25.46734
## 8    Al 2.405394  1.311043 23.61358
## 9    Al 2.424249  1.307667 26.14005
## 10   Al 2.470223  1.223894 21.12235
## 316   H 4.248102  2.362059 11.48540
## 317   H 3.089449  1.235650 11.50871
## 318   O 5.198175 -1.215954 11.52214
## 319   H 4.316270 -1.484605 11.82191
## 320   H 5.855927 -1.641254 12.11139
## 321   O 1.729188 -1.401713 17.91389
## 322   H 2.449020 -2.150314 17.78606
## 323   H 1.984404 -0.578421 17.47553
## 324 322       NA        NA       NA
## 325  Al 0.066718 -0.068740 27.99578
## 326  Al 0.022244 -0.060454 23.60844
```

5.2 Extract data from the raw data frame & cleanning

```
num_fr<-nrow(data_book)/323
temp<-data.frame()
coord_datalist<-list()
for(i in 1:num_fr){
  hd<-270+323*(i-1)
  ta<-323*i
  temp<-data_book[hd:ta,]
  rownames(temp)<-c(1:54)
  coord_datalist[[i]]<-temp
}
coord_data<-array(coord_datalist[])
rm(hd,ta,coord_datalist,temp)
```

5.3 Build density data frame (kg/m3 or g/ml)

```
inters_area=sinpi(1/3)*9.516^2
#10 segments (z from 10 to 20) unit: Angstrom
z_seg=c("10-11","11-12","12-13","13-14","14-15",
        "15-16","16-17","17-18","18-19","19-20")
z_den=data.frame()
temp<-c(0.,0.,0.,0.,0.,0.,0.,0.,0.,0.)
for(n in 1:num_fr){
  for(i in 10:19){
    for(j in 1:54){
      if(coord_data[[n]]$z[j]>i&&coord_data[[1]]$z[j]<=i+1){
        if(coord_data[[n]]$ID[j]=="O")temp[i-9]<-temp[i-9]+15.999/inters_area*10/6.02
        else temp[i-9]<-temp[i-9]+1.007/inters_area*10/6.02
      }
    }
  }
  #make data frame
```

```r
  z_den<-rbind(z_den,temp)
  temp<-c(0.,0.,0.,0.,0.,0.,0.,0.,0.,0.)
}
colnames(z_den)<-z_seg
options(digits = 3)
z_den[1:10,]
```

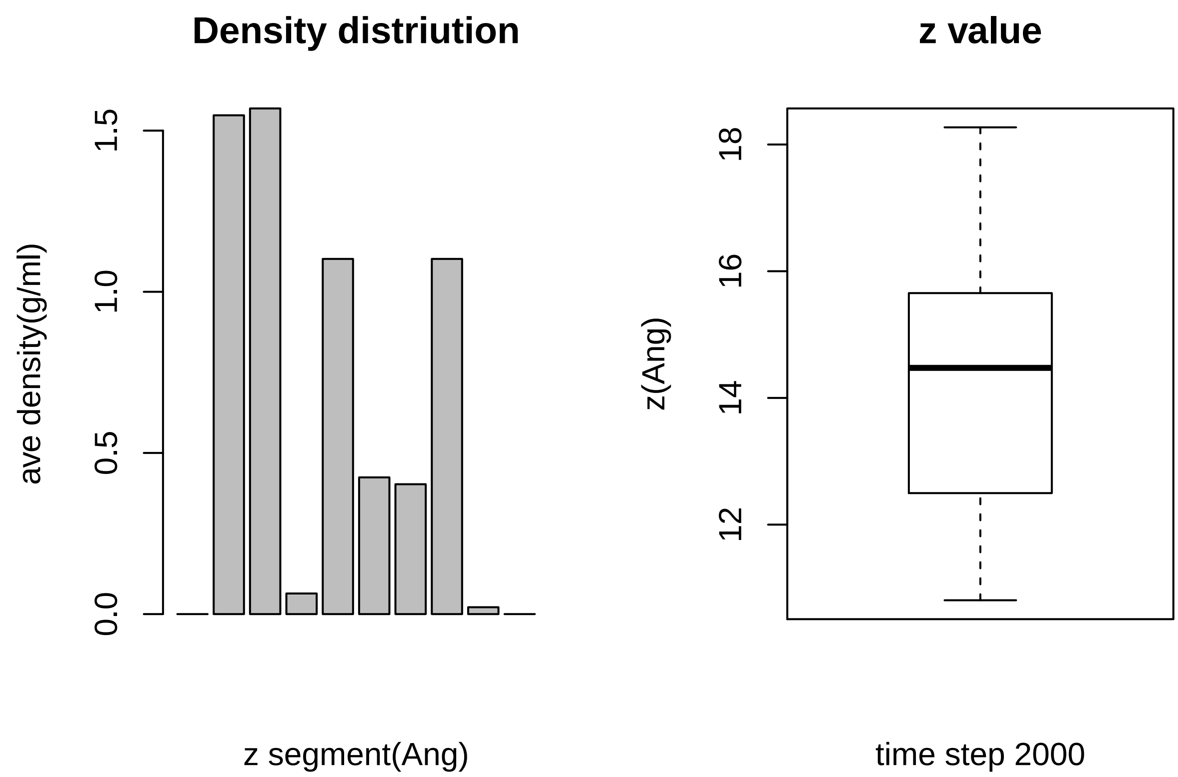
```
##    10-11 11-12 12-13 13-14 14-15 15-16 16-17 17-18 18-19 19-20
## 1      0  1.55 0.742 0.382  1.17   1.1 0.784  1.14     0     0
## 2      0  1.53 0.742 0.382  1.17   1.1 0.784  1.14     0     0
## 3      0  1.50 0.742 0.382  1.17   1.1 0.784  1.14     0     0
## 4      0  1.50 0.742 0.382  1.17   1.1 0.784  1.14     0     0
## 5      0  1.50 0.742 0.382  1.17   1.1 0.784  1.14     0     0
## 6      0  1.50 0.742 0.382  1.17   1.1 0.784  1.14     0     0
## 7      0  1.50 0.742 0.382  1.14   1.1 0.784  1.14     0     0
## 8      0  1.50 0.742 0.403  1.14   1.1 0.784  1.14     0     0
## 9      0  1.50 0.742 0.403  1.14   1.1 0.784  1.14     0     0
## 10     0  1.50 0.742 0.403  1.17   1.1 0.784  1.14     0     0
```

```r
rm(temp)
```

6 Data visualization

Simple data visualization on density ditribution and Z position of atoms for one time step.

```r
x=array(dim = 10)
for(i in 1:10)x[i]<-z_den[2000,i]
par(mfrow=c(1,2))
barplot(x,main = "Density distriution",
        xlab = "z segment(Ang)",ylab = "ave density(g/ml)")
boxplot(coord_data[[2000]]$z,main="z value", xlab="time step 2000",ylab="z(Ang)")
```



7 Exploratory data analysis & interpret results

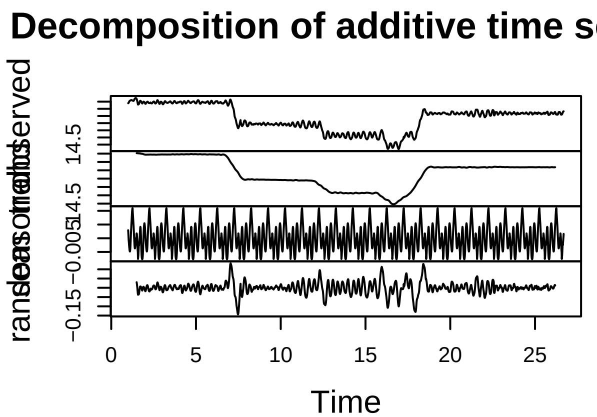
7.1 load data

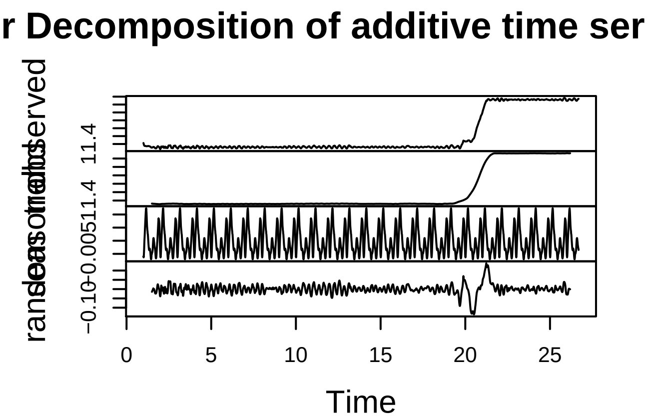
```
data_book<-read.csv("../../data/databook1.csv")
num_fr<-nrow(data_book)/323
temp<-data.frame()
coord_datalist<-list()
for(i in 1:num_fr){
  hd<-270+323*(i-1)
  ta<-323*i
  temp<-data_book[hd:ta,]
  rownames(temp)<-c(1:54)
  coord_datalist[[i]]<-temp
}
coord_data<-array(coord_datalist[])
rm(hd,ta,coord_datalist,temp)
```

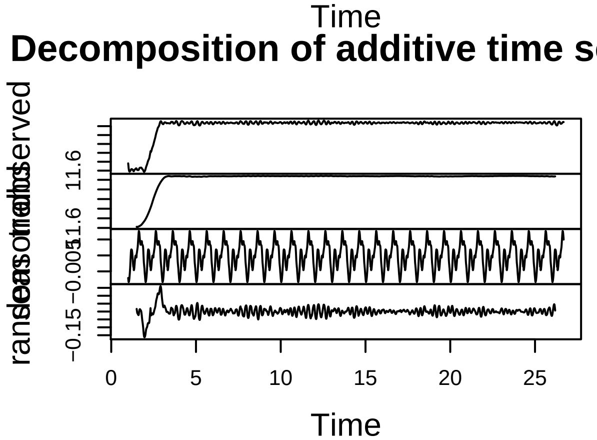
```
Zdistr<-data.frame()
for(j in 1:18){
  for(i in 1:num_fr){
    t<-(coord_data[[i]]$z[3*j-2])
    Zdistr[i,j]<-t
  }
}
```

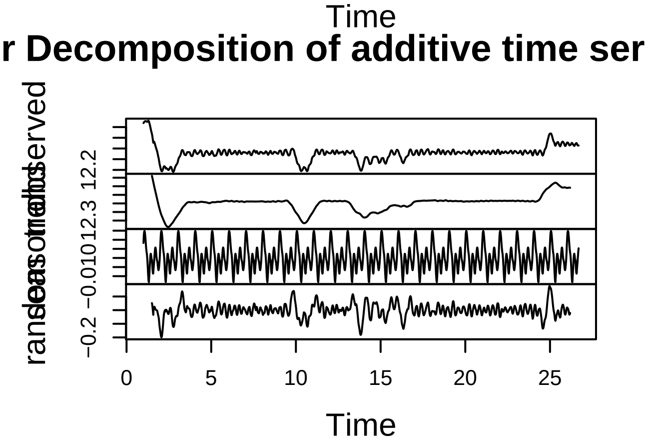
7.2 tsa analysis

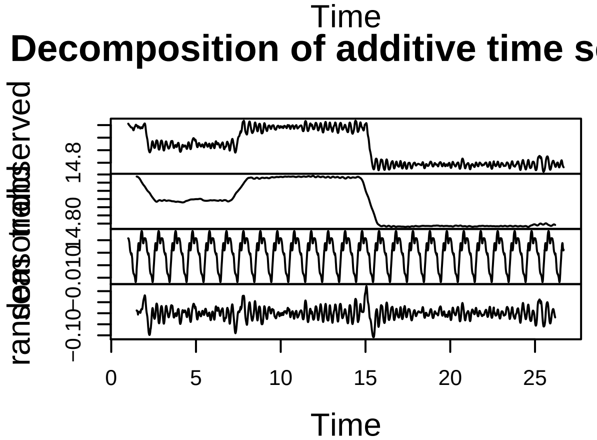
```
tsa_O<-list()
for(i in 1:18){
  tsa_O[[i]]<-decompose(x = ts(data = Zdistr[,i],frequency = 100))
  plot(tsa_O[[i]])
}
```

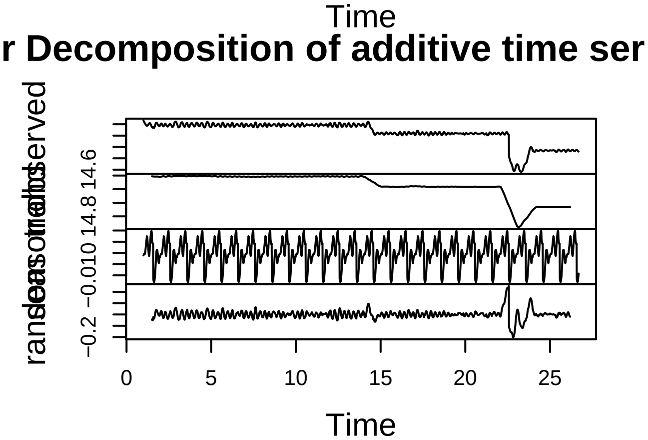


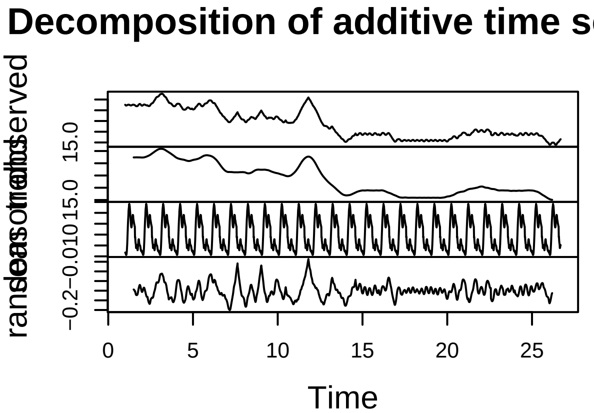


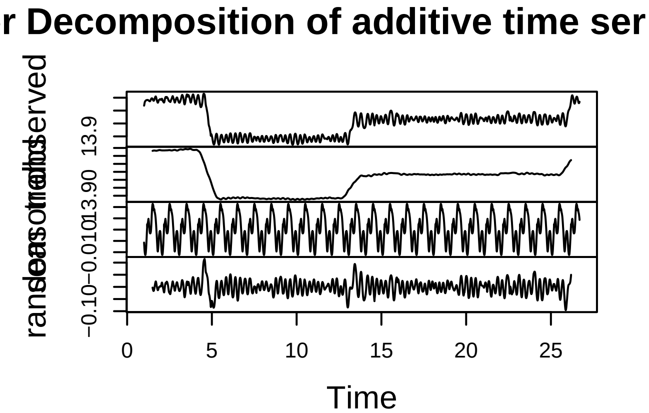


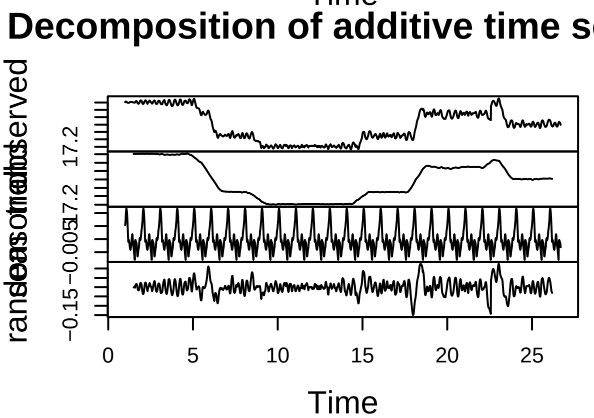


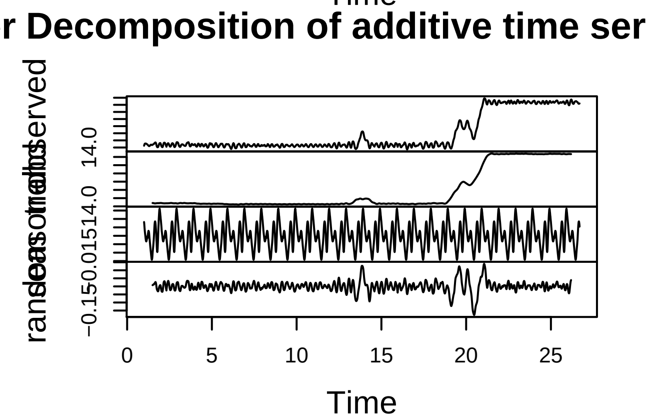


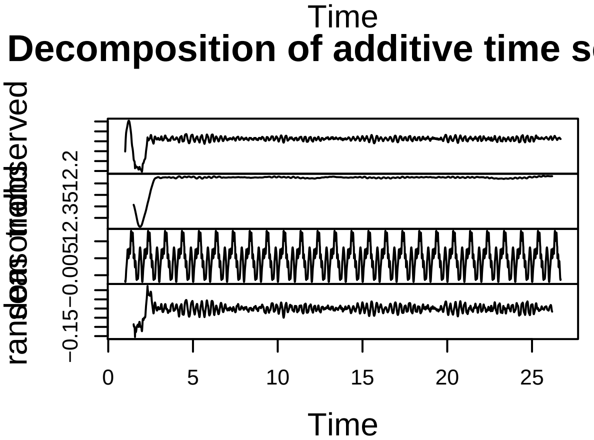


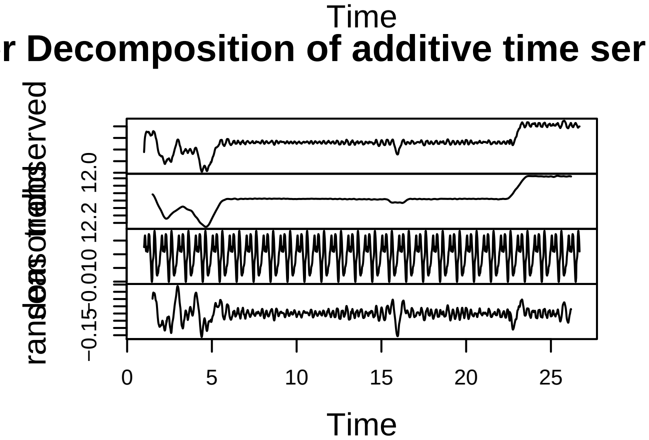

Decomposition of additive time ser
0 5 10 15 20 25
Time

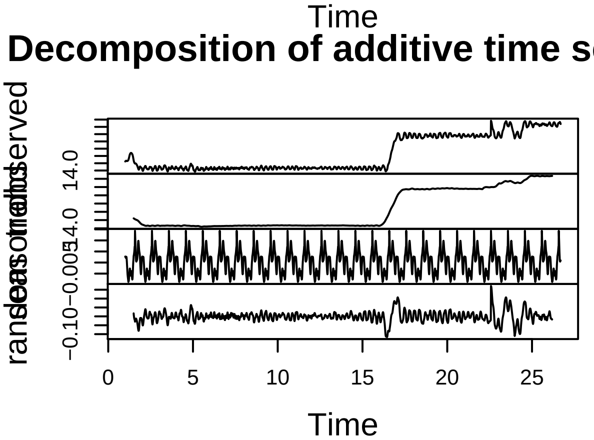

Decomposition of additive time ser
0 5 10 15 20 25
Time

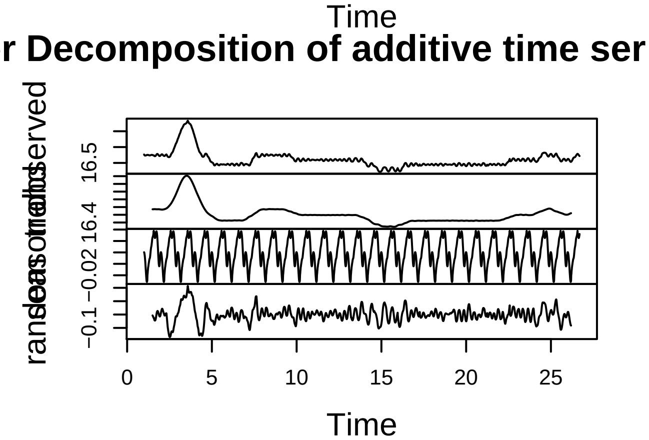

Decomposition of additive time ser
0 5 10 15 20 25
Time

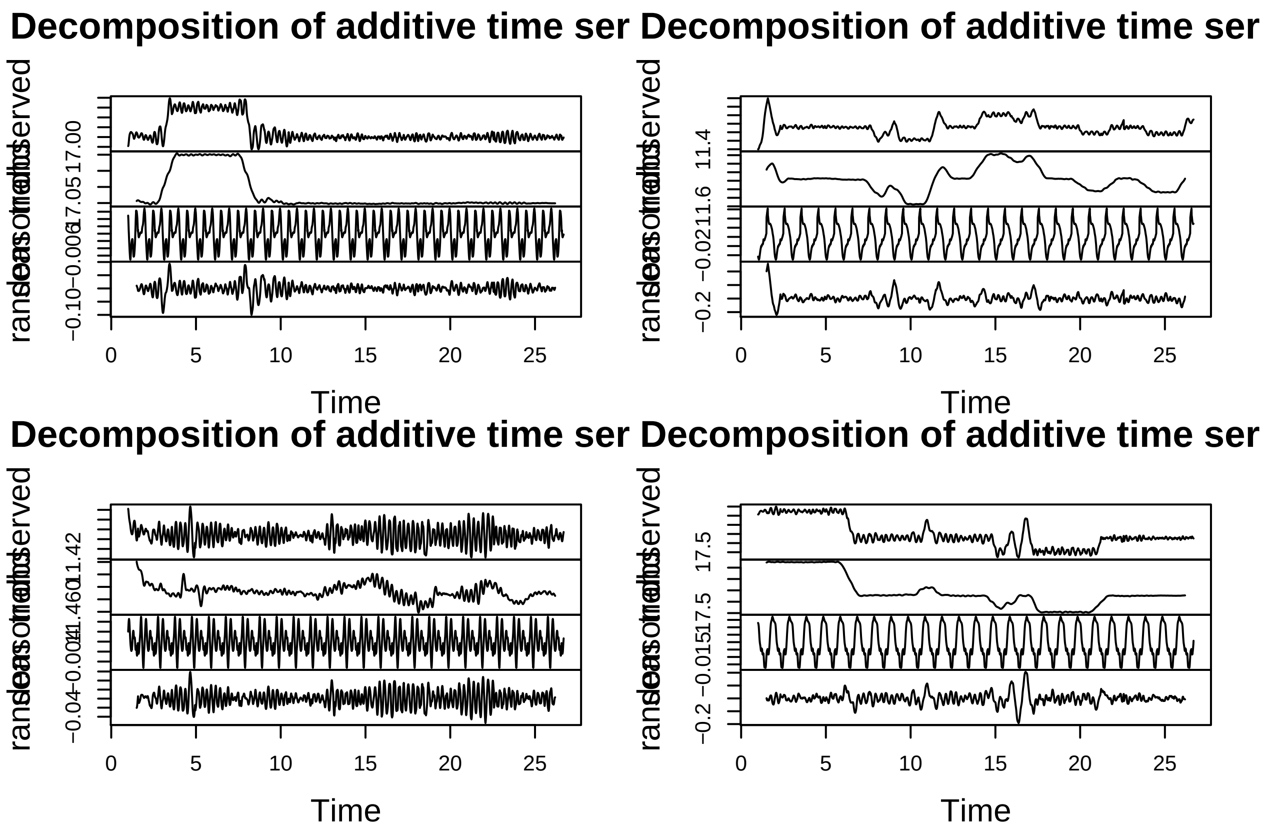

Decomposition of additive time ser
0 5 10 15 20 25
Time


Decomposition of additive time ser
0 5 10 15 20 25
Time


Decomposition of additive time ser
0 5 10 15 20 25
Time


Decomposition of additive time ser
0 5 10 15 20 25
Time


Decomposition of additive time ser
0 5 10 15 20 25
Time

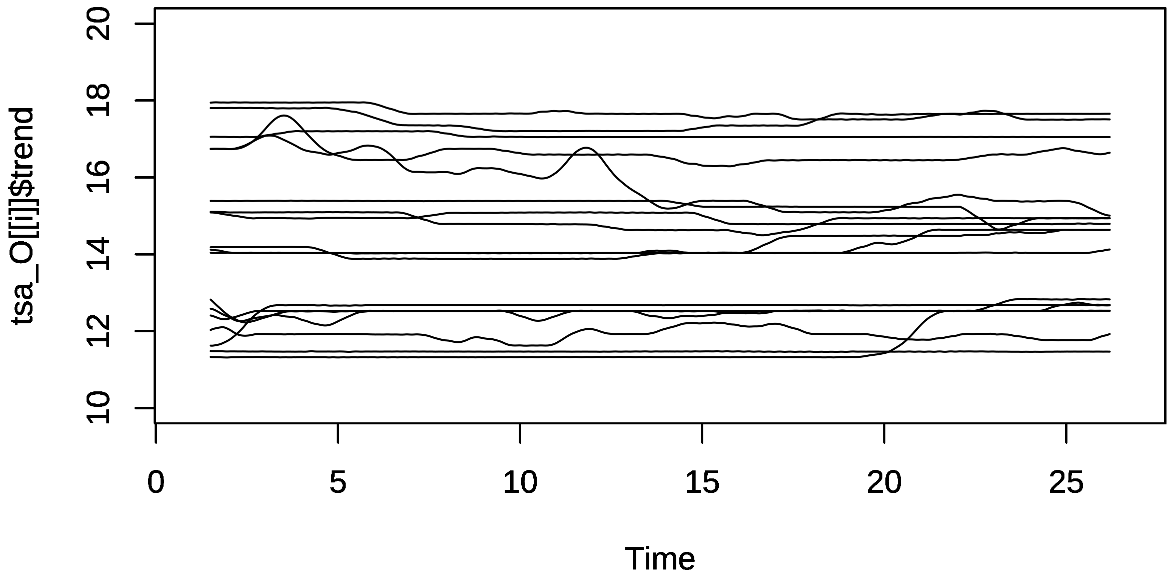


7.3 Z-distribution interpret results

The z-distribution of water molecules was indicated using the Z-values of each oxygen atoms. Since each of the oxygen atoms were associated with a particular water molecule, the movement of water molecules could also be determined by tracking the oxygen atoms. The data obtained in the first part of this project shows the position of each atom at each time and was organized by time.

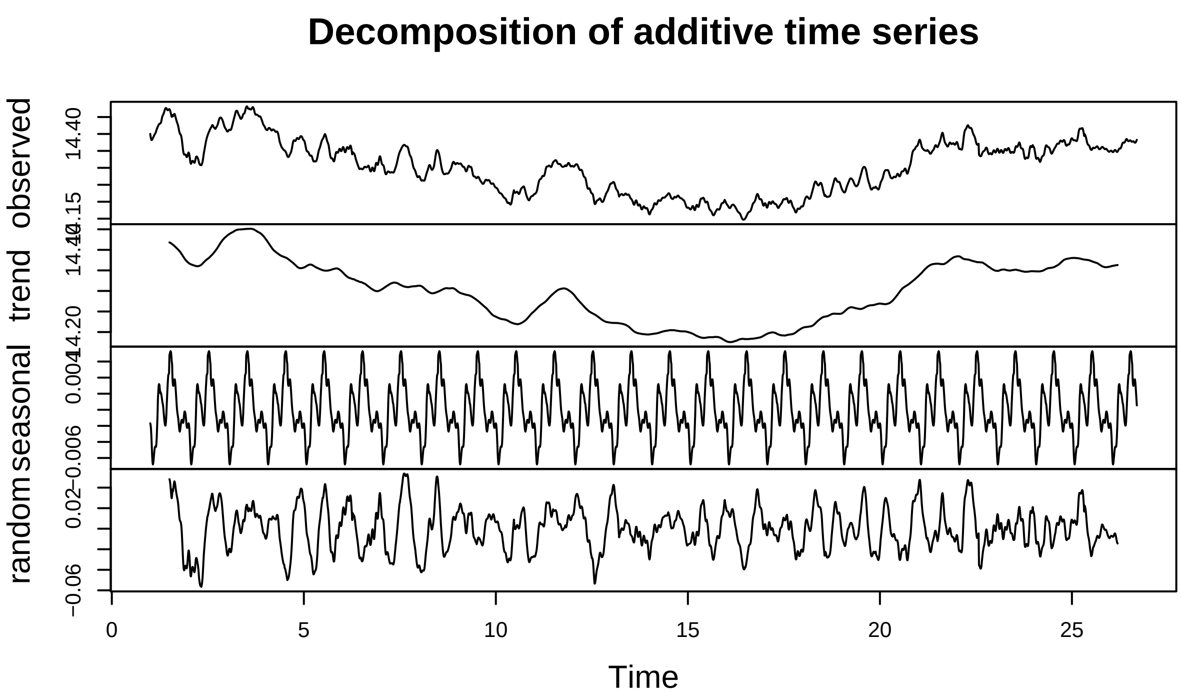
The first thing I looked into is the result given by time series analysis on the coordinate data of 18 oxygen representing the 18 water molecules involved. The graphs given by classical decomposing of the 18 time series could provide a basic idea of the movement of water molecules in there local domains. By looking at the trend plot of each oxygen I could easily conclude that some of the molecules remains where they were original placed during the whole period while most of the waters have to some degree traveled towards the lower or upper plate.

```
for(i in 1:18){
  par(new=T)
  plot(tsa_O[[i]]$trend,ylim=range(10,20))
}
```

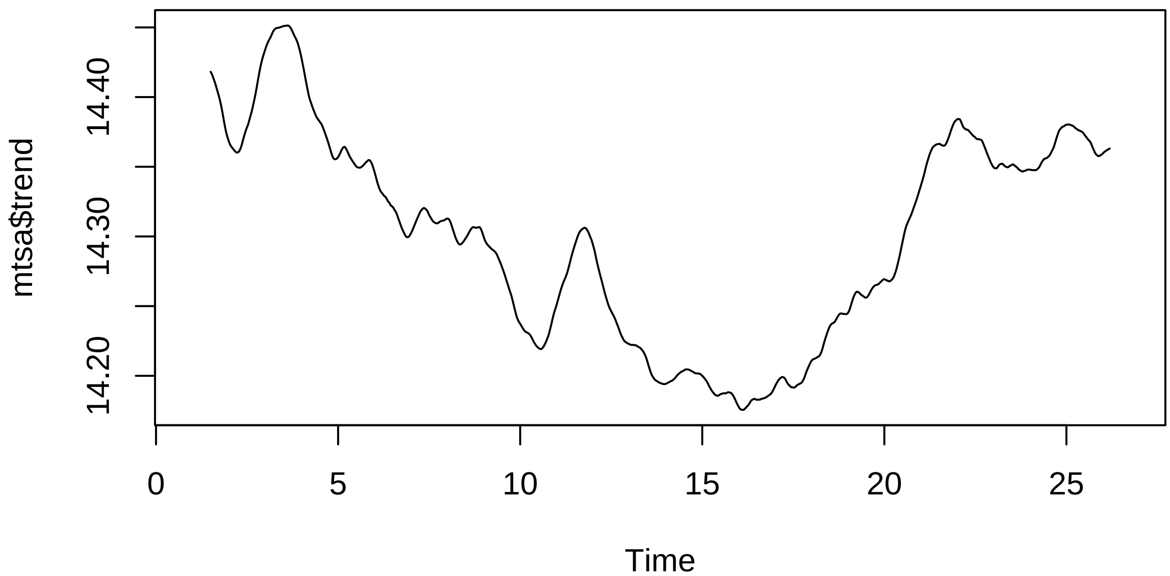


However, these plots are “local”. To show the change of distribution over time I need to put these local information together. So the next thing I plot was a combined plot of these trend components with same scale which contains the z-position and traveling path of the 18 water molecules. From this combined plot, I got an interesting observation that the water molecules were accumulating at a section at z between 12 and 15 leaving only a few water molecules to fill the large space at z from 15 to 19. The water molecules were distributed unevenly.

```
Zmeandistr<-data.frame()
  for(i in 1:num_fr){
    t<-mean(coord_data[[i]]$z)
    Zmeandistr[i,1]<-t
  }
mtsa<-decompose(x = ts(data = Zmeandistr,frequency = 100))
plot(mtsa)
```



```
plot(mtsa$trend)
```

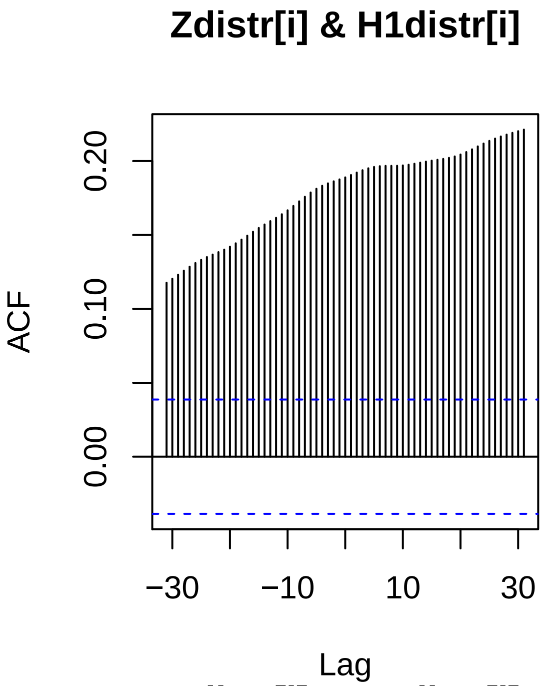


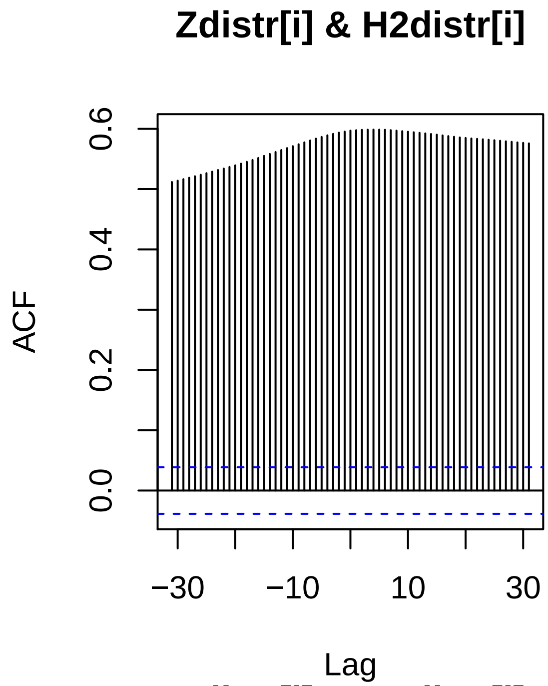
In addition, I did the same analysis on the mean value of z coordinate. As is shown in these plots, the mean value was first decreased and then increased to about 14.35. This again confirmed that the atoms were moving downwards at the fist 2/3 of the time period and then moved back a little.

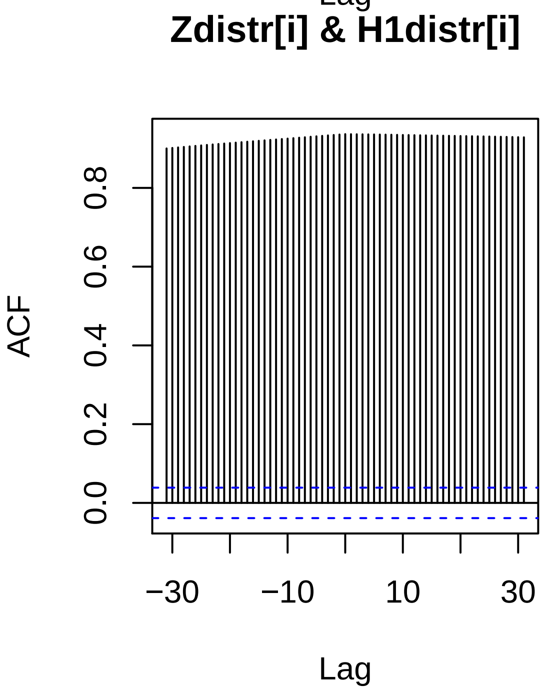
7.4 Correlation interpret results

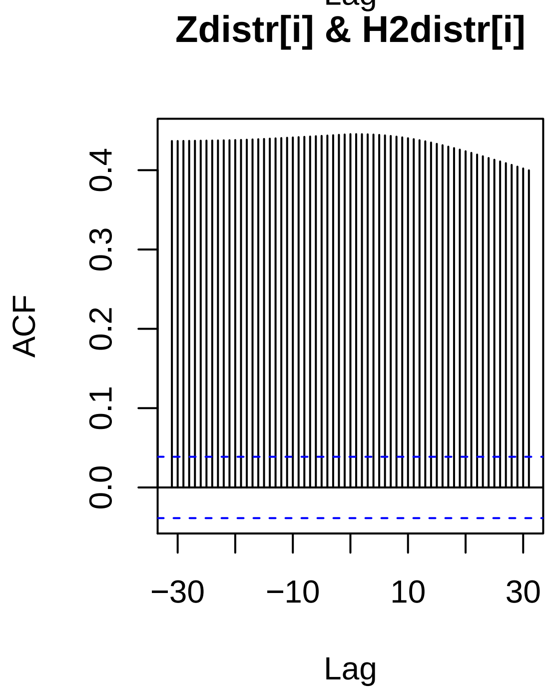
The next important point I'm interested in is dissociation of water molecules. If the water molecule was not dissociated the coordinate data for the oxygen atom and two Hydrogen atoms would be correlated. To check the correlations, cross correlation function estimation was used to calculate the correlation of two series.

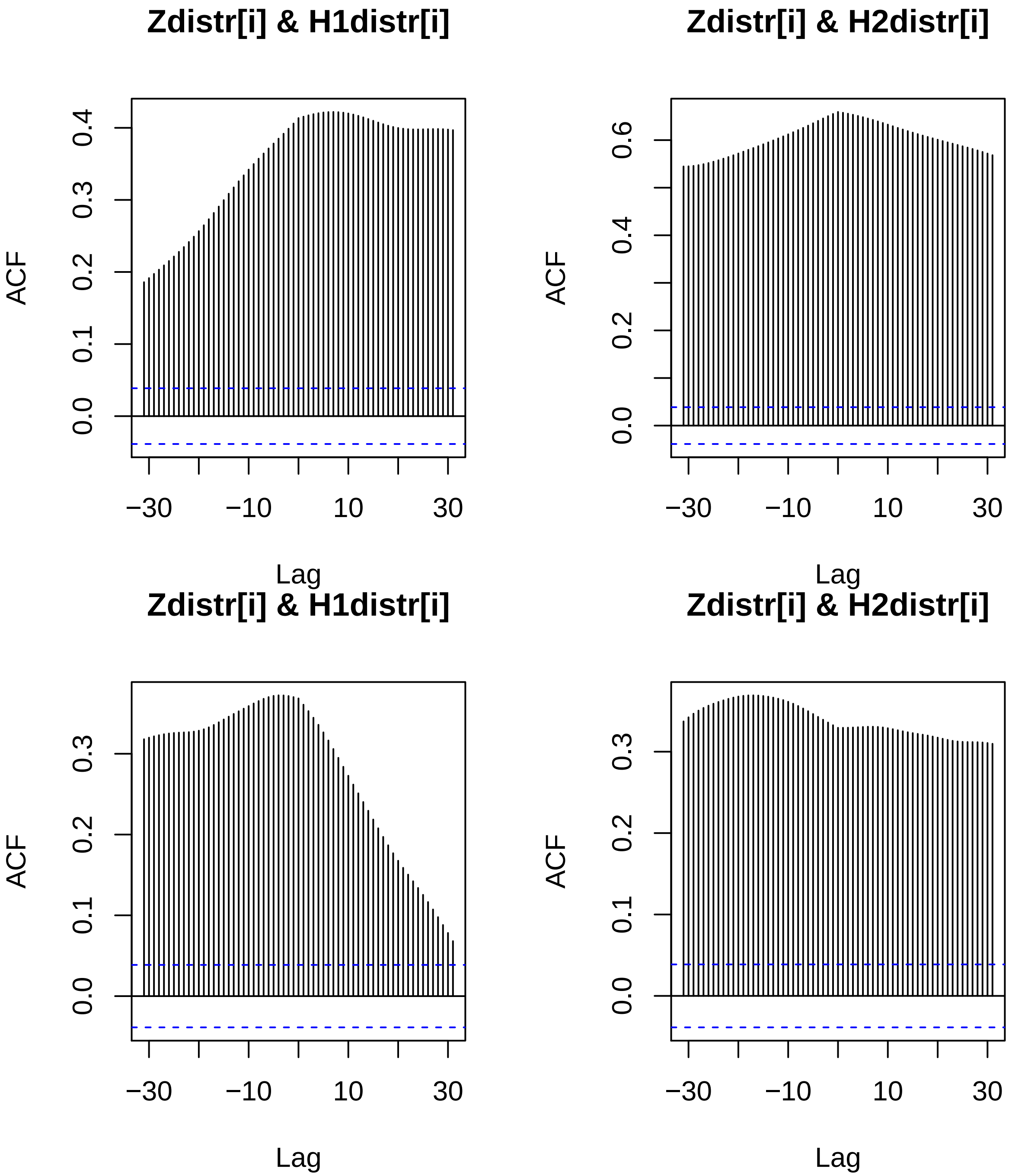
```
H1distr<-data.frame()
for(j in 1:18){
  for(i in 1:num_fr){
    t<-(coord_data[[i]]$z[3*j-1])
    H1distr[i,j]<-t
  }
}
H2distr<-data.frame()
for(j in 1:18){
  for(i in 1:num_fr){
    t<-(coord_data[[i]]$z[3*j])
    H2distr[i,j]<-t
  }
}

for(i in 1:18){
    par(mfrow = c(1, 2))
    ccf(Zdistr[i],H1distr[i])
    ccf(Zdistr[i],H2distr[i])
}
```


Zdistr[i] & H1distr[i]
ACF
0.00
0.10
0.20
−30
−10
10
30
Lag

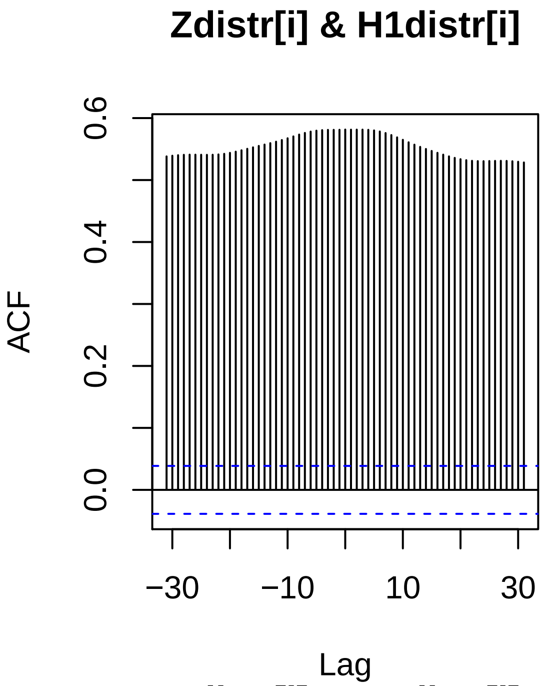

Zdistr[i] & H2distr[i]
ACF
0.0
0.2
0.4
0.6
−30
−10
10
30
Lag

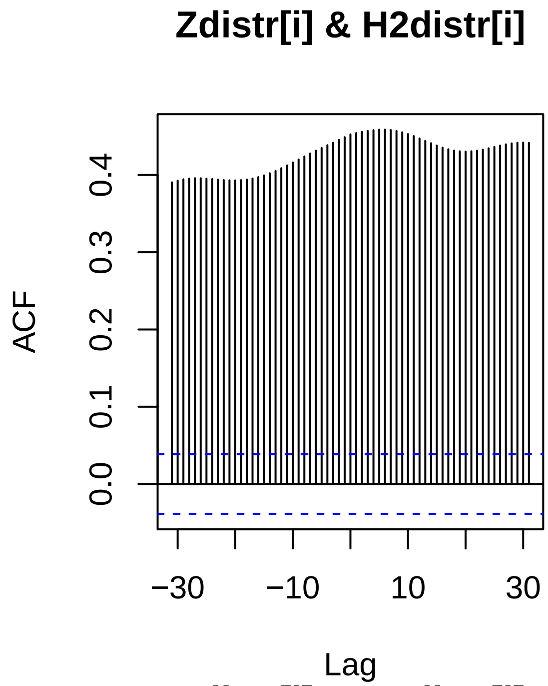

Zdistr[i] & H1distr[i]
ACF
0.0
0.2
0.4
0.6
0.8
−30
−10
10
30
Lag

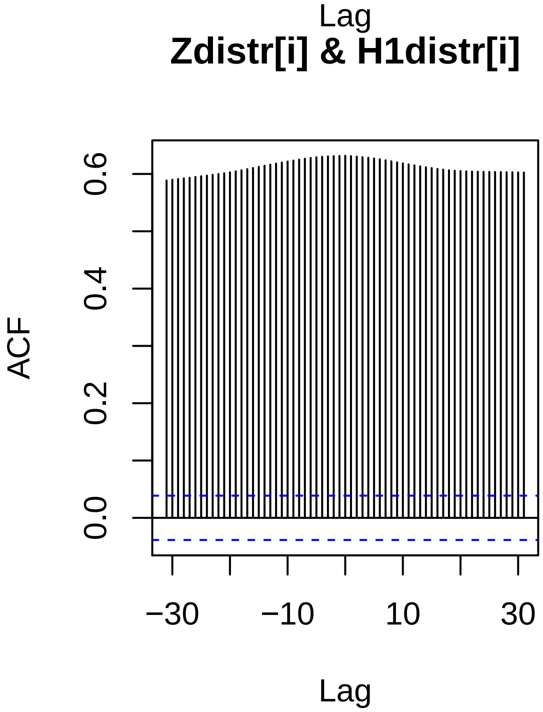

Zdistr[i] & H2distr[i]
ACF
0.0
0.1
0.2
0.3
0.4
−30
−10
10
30
Lag

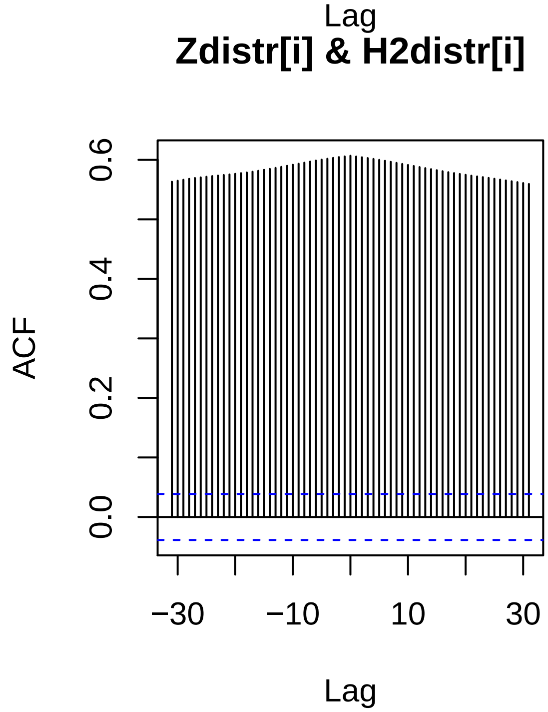


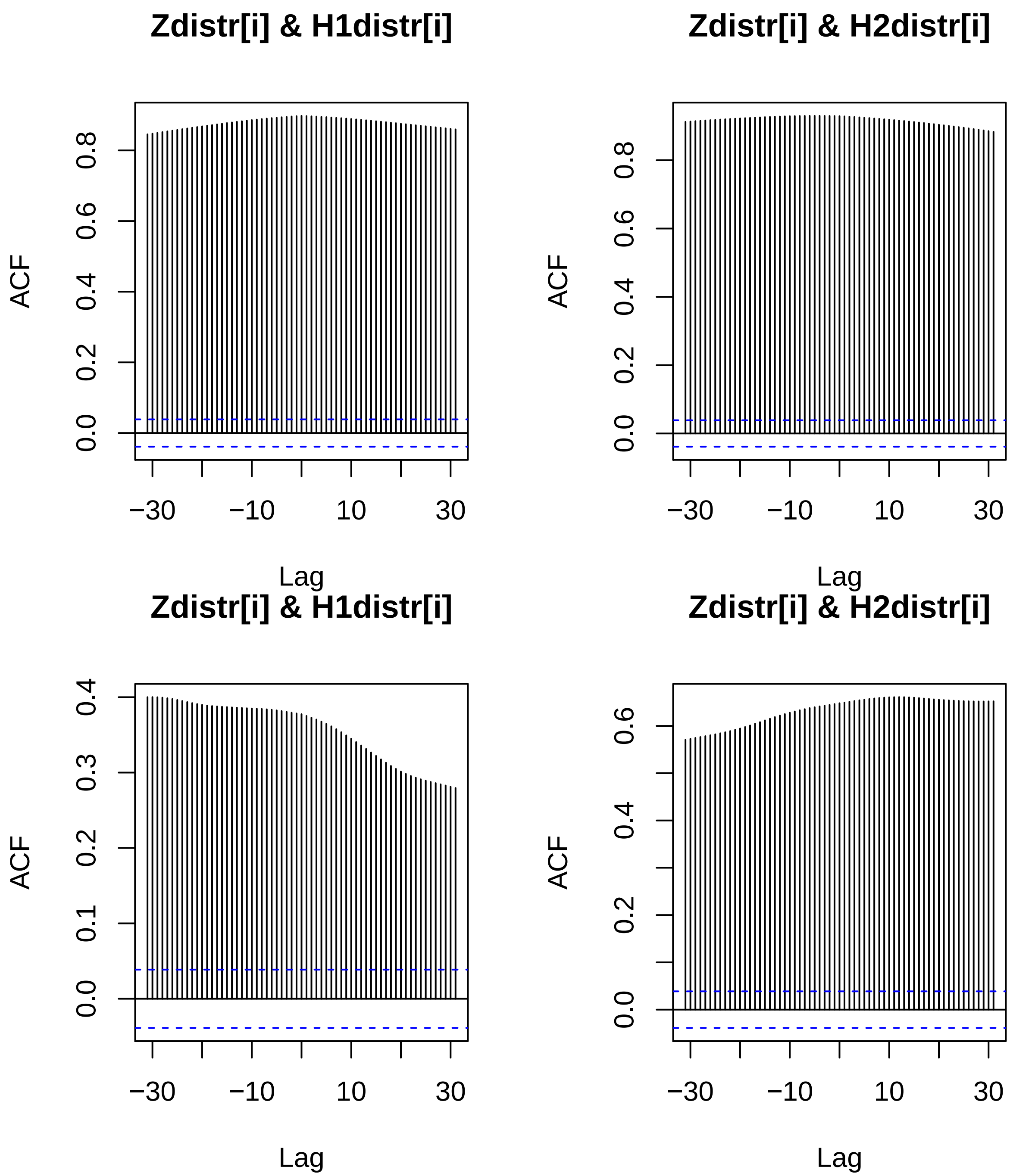
Zdistr[i] & H1distr[i]
Zdistr[i] & H2distr[i]
ACF
Lag
Zdistr[i] & H1distr[i]
Zdistr[i] & H2distr[i]
ACF
Lag

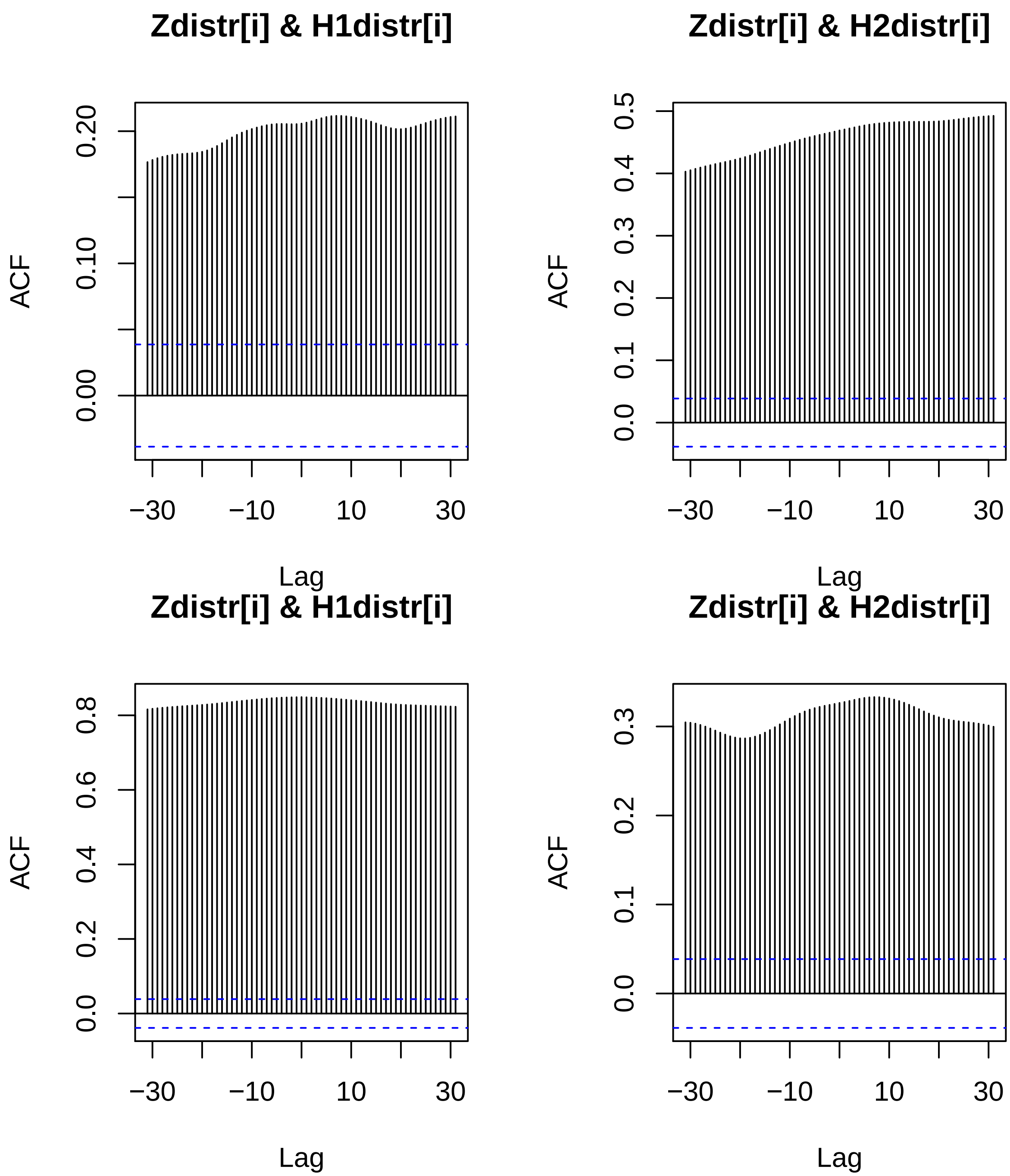

Zdistr[i] & H1distr[i]
ACF
0.0
0.2
0.4
0.6
−30
−10
10
30
Lag

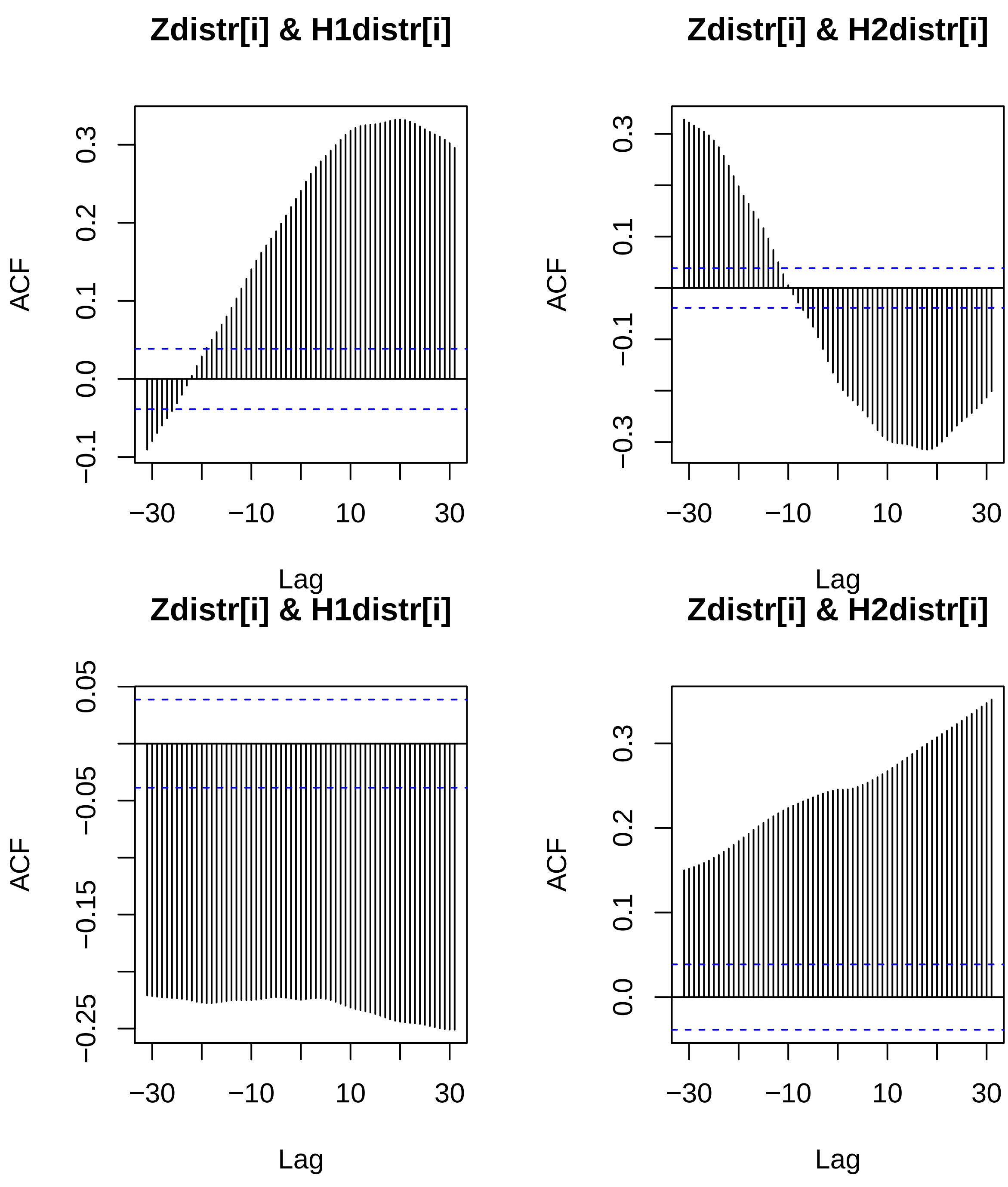

Zdistr[i] & H2distr[i]
ACF
0.0
0.1
0.2
0.3
0.4
−30
−10
10
30
Lag

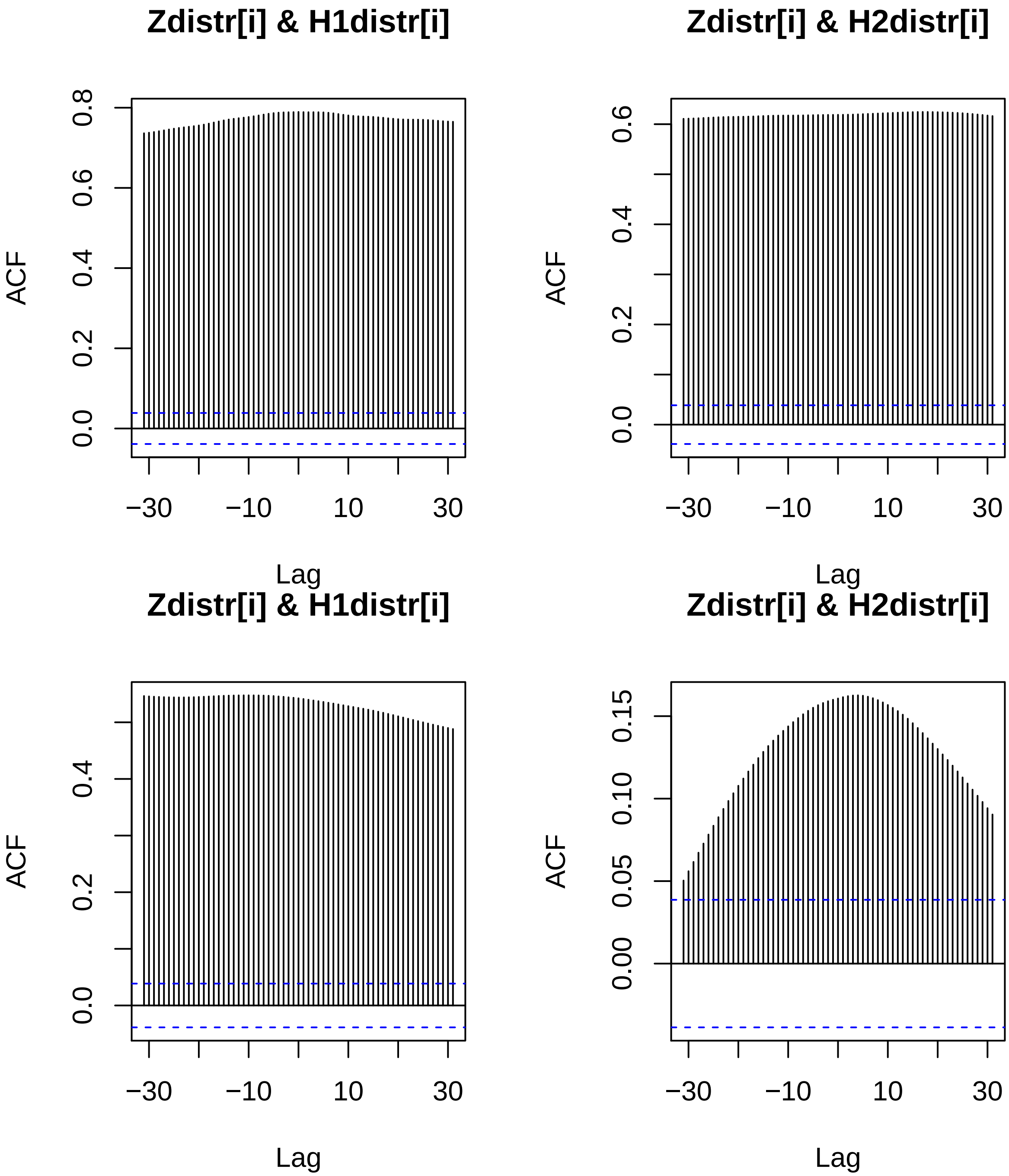

Zdistr[i] & H1distr[i]
ACF
0.0
0.2
0.4
0.6
−30
−10
10
30
Lag

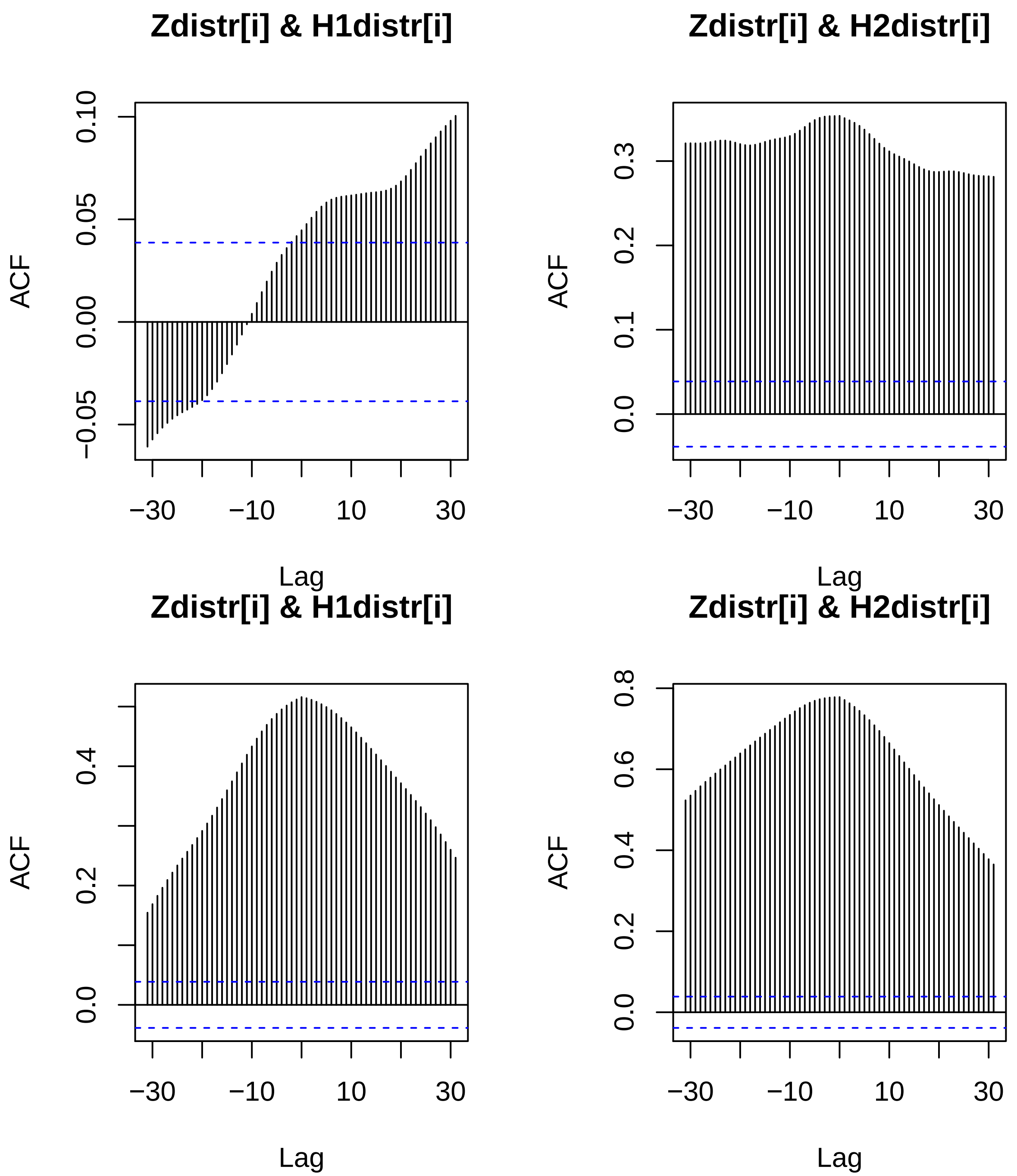

Zdistr[i] & H2distr[i]
ACF
0.0
0.2
0.4
0.6
−30
−10
10
30
Lag

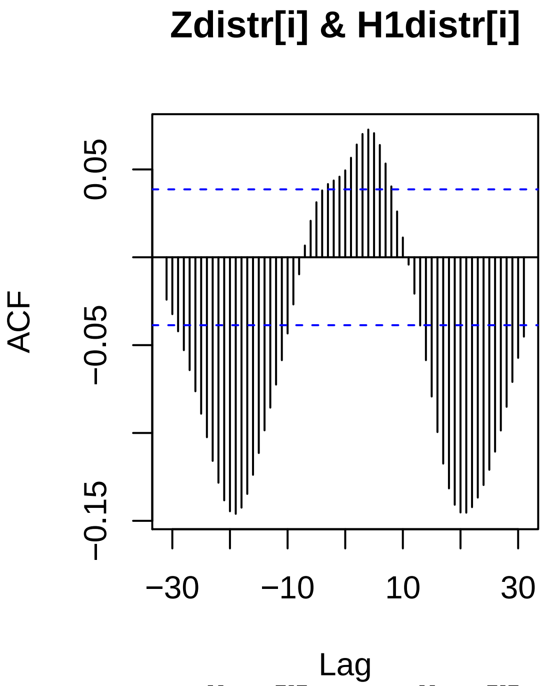

Zdistr[i] & H1distr[i]
Zdistr[i] & H2distr[i]
Zdistr[i] & H1distr[i]
Zdistr[i] & H2distr[i]
ACF
Lag
0.0
0.2
0.4
0.6
0.8
0.1
0.3
−30
−10
10
30

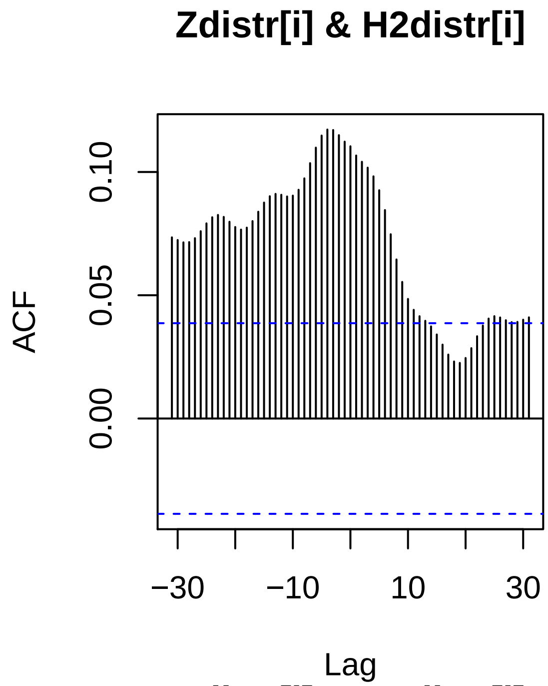

Zdistr[i] & H1distr[i]
ACF
0.00
0.10
0.20
−30
−10
10
30
Lag
Zdistr[i] & H2distr[i]
ACF
0.0
0.1
0.2
0.3
0.4
0.5
−30
−10
10
30
Lag
Zdistr[i] & H1distr[i]
ACF
0.0
0.2
0.4
0.6
0.8
−30
−10
10
30
Lag
Zdistr[i] & H2distr[i]
ACF
0.0
0.1
0.2
0.3
−30
−10
10
30
Lag

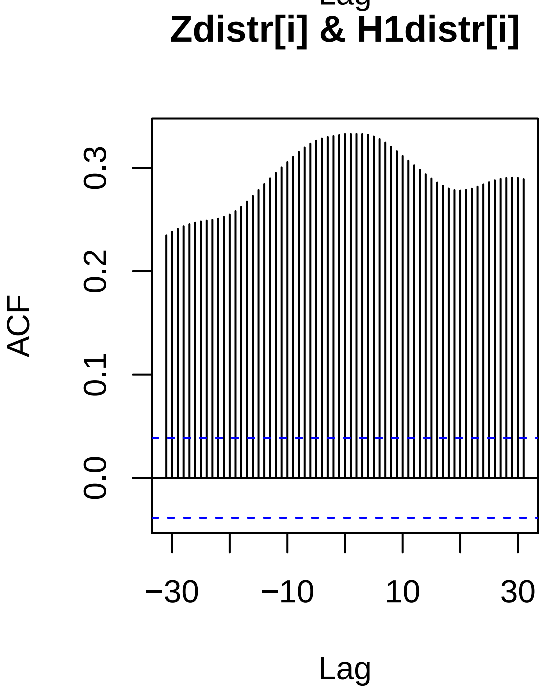

Zdistr[i] & H1distr[i]
Zdistr[i] & H2distr[i]
Zdistr[i] & H1distr[i]
Zdistr[i] & H2distr[i]
ACF
Lag
−30
−10
10
30
0.3
0.2
0.1
0.0
−0.1
−0.3
0.05
−0.05
−0.15
−0.25

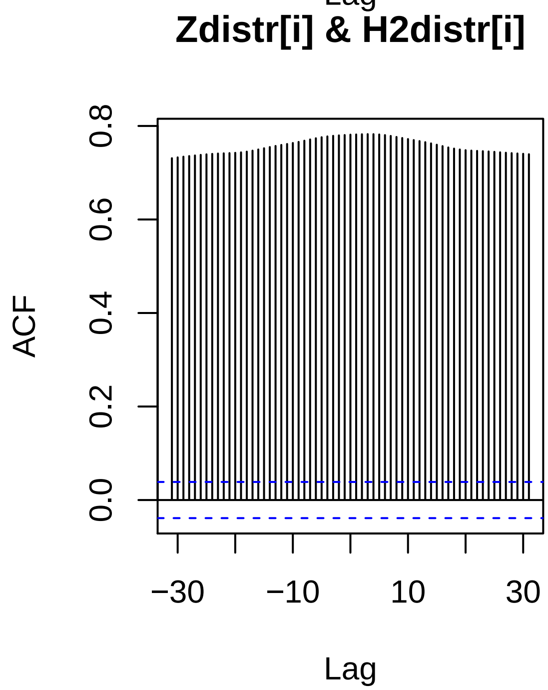

Zdistr[i] & H1distr[i]
Zdistr[i] & H2distr[i]
Zdistr[i] & H1distr[i]
Zdistr[i] & H2distr[i]
ACF
Lag
−30
−10
10
30
0.0
0.2
0.4
0.6
0.8
0.00
0.05
0.10
0.15


Zdistr[i] & H1distr[i]
ACF
−0.05
0.00
0.05
0.10
−30
−10
10
30
Lag
Zdistr[i] & H2distr[i]
ACF
0.0
0.1
0.2
0.3
−30
−10
10
30
Lag
Zdistr[i] & H1distr[i]
ACF
0.0
0.2
0.4
−30
−10
10
30
Lag
Zdistr[i] & H2distr[i]
ACF
0.0
0.2
0.4
0.6
0.8
−30
−10
10
30
Lag





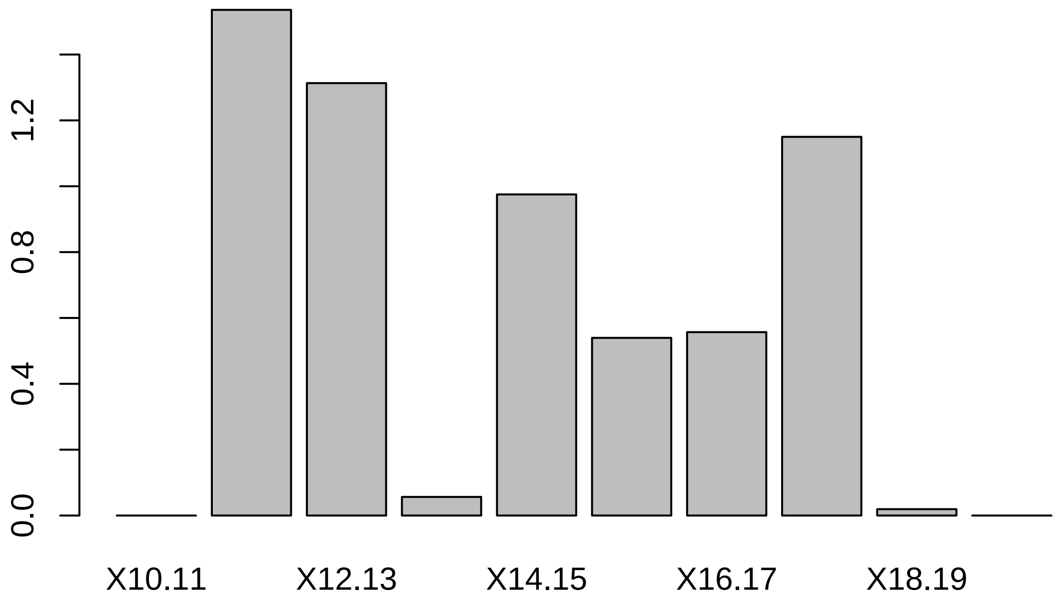




These plots shows the results of the estimation of the auto correlation function. By interpreting these plots, most of water molecules were not dissociated. The correlation were above the confidence interval which indicates that the movement of two H atoms were correlated to that of the Oxygen atom in the center. However there are several plots that shows a different result. Take the 33rd plot as an example, the correlation between the Oxygen and Hydrogen atoms was weak and only exists at lag from -30 to 10 so it was likely that this water molecule was deformed.

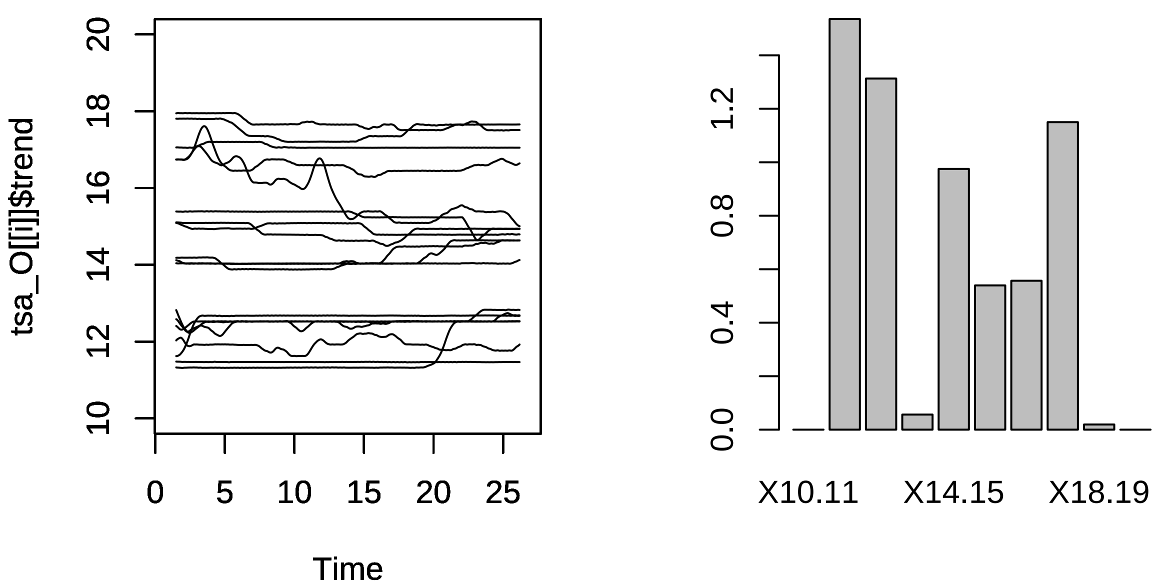
7.5 density distribution

```
dendata<-read.csv("../../data/data.csv")
dendata<-dendata[,c(2:11)]
barplot(colMeans(dendata))
```



By comparing the trend plot and the mean density plot, it seems that there was a blank space in z between 13 and 14 that water molecules were neither went into or went through it. Moreover while almost no water molecules were inside this slot water molecules were accumulated on both sides.

```
par(mfrow=c(1,2))
for(i in 1:18){
  par(new=T)
  plot(tsa_O[[i]]$trend,ylim=range(10,20))
}
barplot(colMeans(dendata))
```



A possible explanation would be the water has two layers and the interface of the two layer appears in somewhere between z=13 and z=14. And notice that the density in both layers were quite different compared to the usual water density, the water molecules here are not liquid water which is reasonable since these water molecules represents the moisture brought into the system from the air. When the surfaces of two materials were close to each other these water molecules in between will not be in the normal phase typically the density would be less than 1. In this particular case, though the overall density calculated was less than 1, the layer close to the lower plate (quartz) was much denser and thinner which is also accord with the hydrophilic nature of quartz surface.

8 Challenge results

The data was based on a single simulation with the initial position of atoms set in place. However the water molecules' position was generated randomly so there may be different results with a different models as I cannot prove in this project.

The deformation of water molecules were anaylized using the correlation between O and two H that were originaly bonded with it. So it is possible that after one H was dissociated another H took the place.