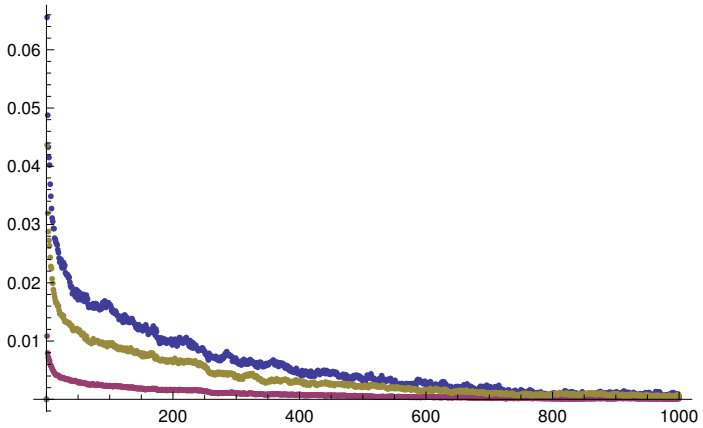
NMR Relaxation of 1H of water molecules

Reading the data files obtained from the MD simulations' trajectories:

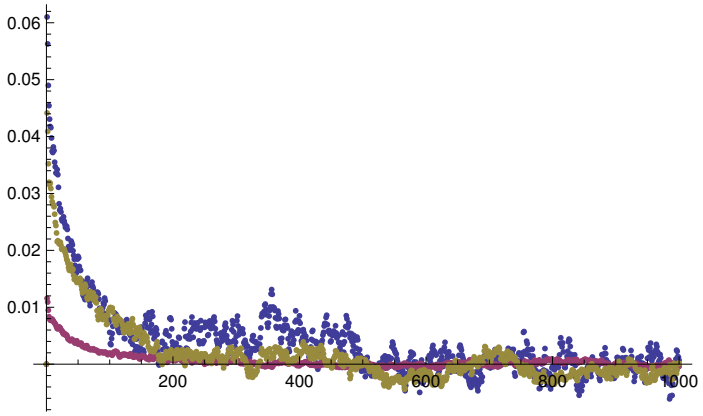
```
factorT1 = 100; (* time scale intermolecular correlation functions in fs*)
factorT2 = 10; (* time scale intramolecular correlation functions in fs*)
listRelaxDipInter = Import[
    "/home/ccalero/Documents/0_RECERCA/Fase_plastica_aigua_NMR_relaxation/Analisi/
      LIQUID/Relaxation_dipolar_intermolecular_npt_all_100.dat"];
coef00DipInter = Table[{listRelaxDipInter[[n + 1, 1]], listRelaxDipInter[[n + 1, 2]]},
    {n, 1, Length[listRelaxDipInter] - 2}];
coef11DipInter = Table[{listRelaxDipInter[[n + 1, 1]], listRelaxDipInter[[n + 1, 3]]},
    {n, 1, Length[listRelaxDipInter] - 2}];
coef22DipInter = Table[{listRelaxDipInter[[n + 1, 1]], listRelaxDipInter[[n + 1, 5]]},
    {n, 1, Length[listRelaxDipInter] - 2}];

listRelaxDipIntra = Import[
    "/home/ccalero/Documents/0_RECERCA/Fase_plastica_aigua_NMR_relaxation/Analisi/
      LIQUID/Relaxation_dipolar_intramolecular_npt_all_10.dat"];
coef00DipIntra = Table[{listRelaxDipIntra[[n + 1, 1]], listRelaxDipIntra[[n + 1, 2]]},
    {n, 1, Length[listRelaxDipIntra] - 2}];
coef11DipIntra = Table[{listRelaxDipIntra[[n + 1, 1]], listRelaxDipIntra[[n + 1, 3]]},
    {n, 1, Length[listRelaxDipIntra] - 2}];
coef22DipIntra = Table[{listRelaxDipIntra[[n + 1, 1]], listRelaxDipIntra[[n + 1, 5]]},
    {n, 1, Length[listRelaxDipIntra] - 2}];


ListPlot[{coef00DipInter, coef11DipInter, coef22DipInter}, PlotRange → All]
```



```
ListPlot[{coef00DipIntra, coef11DipIntra, coef22DipIntra}, PlotRange → All]
```

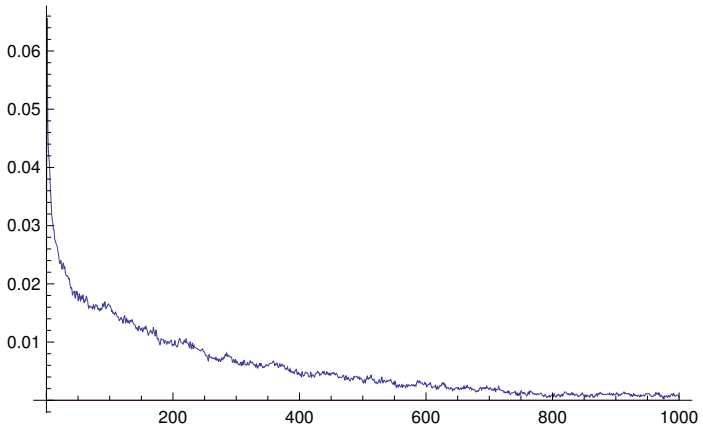


Obtaining interpolating functions and/or fits of the data:

```
Interpolcoef00DipInter = Interpolation[coef00DipInter];
Interpolcoef11DipInter = Interpolation[coef11DipInter];
Interpolcoef22DipInter = Interpolation[coef22DipInter];

Interpolcoef00DipIntra = Interpolation[coef00DipIntra];
Interpolcoef11DipIntra = Interpolation[coef11DipIntra];
Interpolcoef22DipIntra = Interpolation[coef22DipIntra];
```

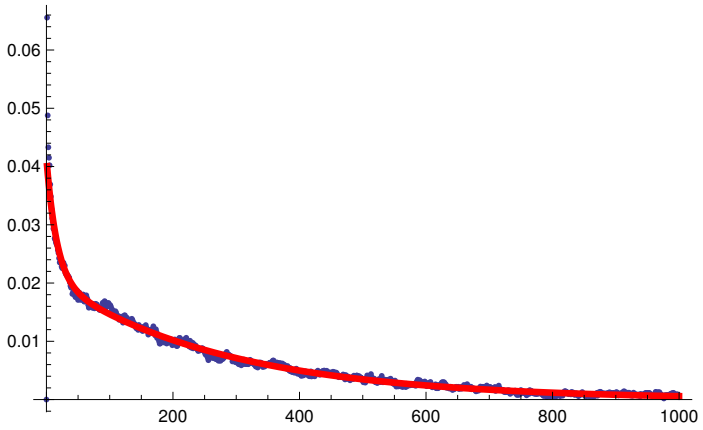
```
Plot[{Interpolcoef00DipInter[x], 0}, {x, 0, 1000}, PlotRange → All]
```



Intermolecular contribution

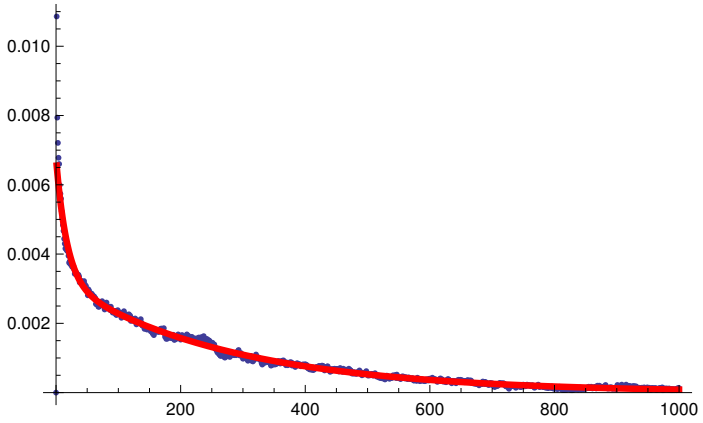
```
resfit00DipInter = FindFit[coef00DipInter,
  {a * Exp[-b * x] + c * Exp[-d * x], a > 0, b > 0, c > 0, d > 0}, {{a, 0.2}, b, c, d}, x]
a00DipInter = a /. resfit00DipInter[[1]]; b00DipInter = b /. resfit00DipInter[[2]];
c00DipInter = c /. resfit00DipInter[[3]];
d00DipInter = d /. resfit00DipInter[[4]];
Fitcoef00DipInter[x_] =
  a00DipInter * Exp[-b00DipInter * x] + c00DipInter * Exp[-d00DipInter * x];
Show[ListPlot[coef00DipInter, PlotRange → All], Plot[Fitcoef00DipInter[x],
  {x, 1, 1000}, PlotRange → {0, 1000}, PlotStyle → {Red, Thickness → 0.01}]]
```

```
{a → 0.020909, b → 0.00359168, c → 0.0204417, d → 0.0618344}
```



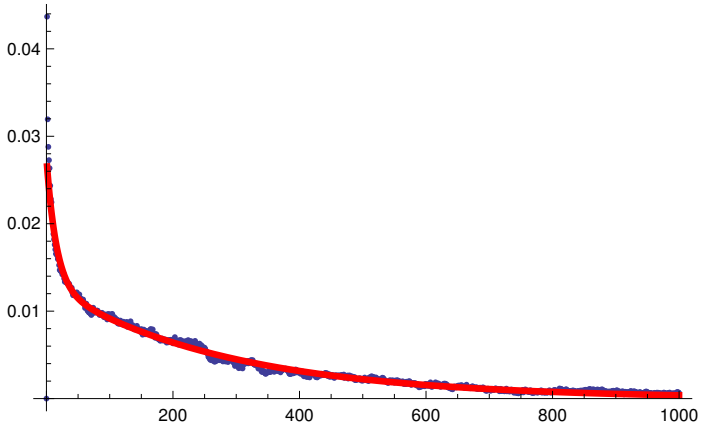
```
resfit11DipInter = FindFit[coef11DipInter,
  {a * Exp[-b * x] + c * Exp[-d * x], a > 0, b > 0, c > 0, d < 1}, {{a, 0.01}, b, c, {d, 0.1}}, x]
a11DipInter = a /. resfit11DipInter[[1]]; b11DipInter = b /. resfit11DipInter[[2]];
c11DipInter = c /. resfit11DipInter[[3]];
d11DipInter = d /. resfit11DipInter[[4]];
Fitcoef11DipInter[x_] =
  a11DipInter * Exp[-b11DipInter * x] + c11DipInter * Exp[-d11DipInter * x];
Show[ListPlot[coef11DipInter, PlotRange → All], Plot[Fitcoef11DipInter[x],
  {x, 1, 1000}, PlotRange → {0, 1000}, PlotStyle → {Red, Thickness → 0.01}]]
```

```
{a → 0.00326756, b → 0.0036475, c → 0.00349448, d → 0.0578977}
```



```
resfit22DipInter = FindFit[coef22DipInter,
  {a * Exp[-b * x] + c * Exp[-d * x], a > 0, b > 0, c > 0, d < 1}, {{a, 0.01}, b, c, {d, 0.02}}, x]
a22DipInter = a /. resfit22DipInter[[1]]; b22DipInter = b /. resfit22DipInter[[2]];
c22DipInter = c /. resfit22DipInter[[3]];
d22DipInter = d /. resfit22DipInter[[4]];
Fitcoef22DipInter[x_] =
  a22DipInter * Exp[-b22DipInter * x] + c22DipInter * Exp[-d22DipInter * x];
Show[ListPlot[coef22DipInter, PlotRange → All], Plot[Fitcoef22DipInter[x],
  {x, 1, 1000}, PlotRange → {0, 1000}, PlotStyle → {Red, Thickness → 0.01}]]
```

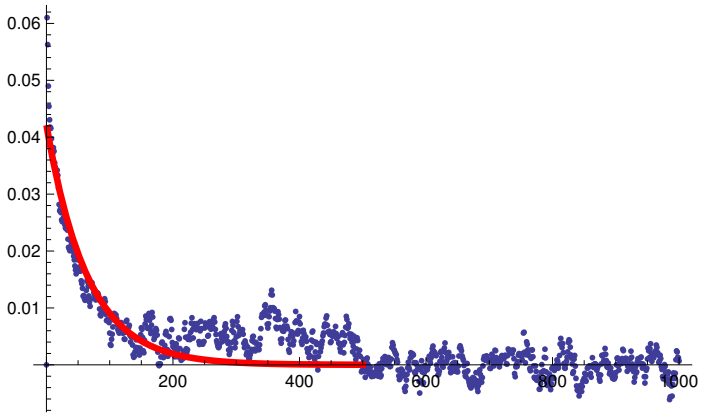
```
{a → 0.0130103, b → 0.00354161, c → 0.0144858, d → 0.0646745}
```



Intramolecular contribution

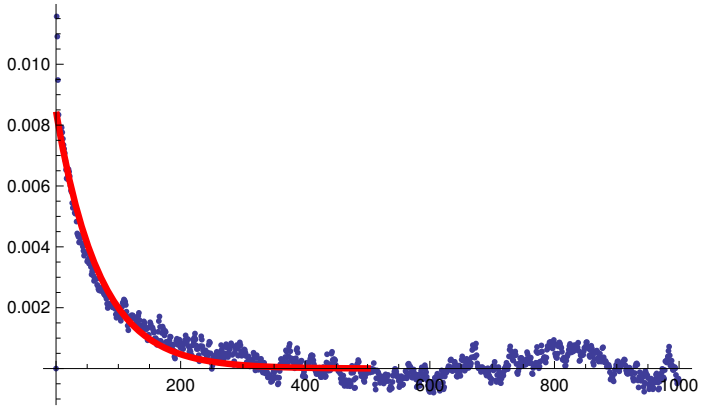
```
resfit00DipIntra =
 FindFit[coef00DipIntra, a * Exp[-b * x] + c * Exp[-d * x], {{a, 0.01}, b, c, {d, 0.02}}, x]
a00DipIntra = a /. resfit00DipIntra[[1]]; b00DipIntra = b /. resfit00DipIntra[[2]];
c00DipIntra = c /. resfit00DipIntra[[3]];
d00DipIntra = d /. resfit00DipIntra[[4]];
Fitcoef00DipIntra[x_] =
  a00DipIntra * Exp[-b00DipIntra * x] + c00DipIntra * Exp[-d00DipIntra * x];
Show[ListPlot[coef00DipIntra, PlotRange → All], Plot[Fitcoef00DipIntra[x],
  {x, 1, 500}, PlotRange → {0, 500}, PlotStyle → {Red, Thickness → 0.01}]]
```

```
{a → -0.0421882, b → 830.019, c → 0.0421882, d → 0.0153943}
```



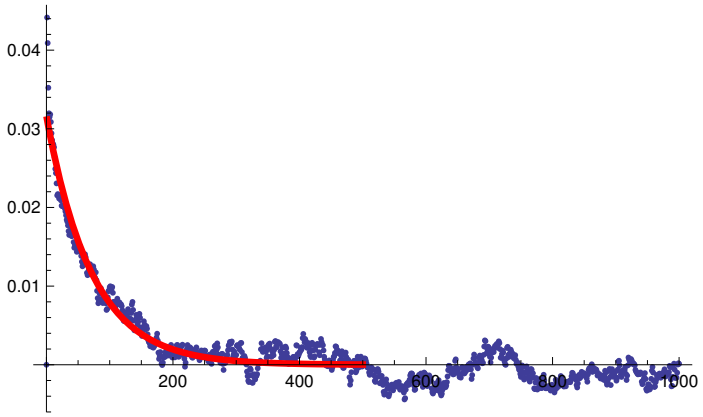
```
resfit11DipIntra =
 FindFit[coef11DipIntra, a * Exp[-b * x] + c * Exp[-d * x], {{a, 0.01}, b, c, {d, 0.02}}, x]
a11DipIntra = a /. resfit11DipIntra[[1]]; b11DipIntra = b /. resfit11DipIntra[[2]];
c11DipIntra = c /. resfit11DipIntra[[3]];
d11DipIntra = d /. resfit11DipIntra[[4]];
Fitcoef11DipIntra[x_] =
  a11DipIntra * Exp[-b11DipIntra * x] + c11DipIntra * Exp[-d11DipIntra * x];
Show[ListPlot[coef11DipIntra, PlotRange → All], Plot[Fitcoef11DipIntra[x],
  {x, 1, 500}, PlotRange → {0, 500}, PlotStyle → {Red, Thickness → 0.01}]]
```

{a → -0.00845793, b → 765.948, c → 0.00845793, d → 0.0144526}




```
resfit22DipIntra =
 FindFit[coef22DipIntra, a * Exp[-b * x] + c * Exp[-d * x], {{a, 0.01}, b, c, {d, 0.02}}, x]
a22DipIntra = a /. resfit22DipIntra[[1]]; b22DipIntra = b /. resfit22DipIntra[[2]];
c22DipIntra = c /. resfit22DipIntra[[3]];
d22DipIntra = d /. resfit22DipIntra[[4]];
Fitcoef22DipIntra[x_] =
  a22DipIntra * Exp[-b22DipIntra * x] + c22DipIntra * Exp[-d22DipIntra * x];
Show[ListPlot[coef22DipIntra, PlotRange → All], Plot[Fitcoef22DipIntra[x],
  {x, 1, 500}, PlotRange → {0, 500}, PlotStyle → {Red, Thickness → 0.01}]]
```

{a → -0.0316113, b → 750.741, c → 0.0316113, d → 0.013936}



Calculation of Spectral functions

```
ω1 = 267.513 * 10^-9 * factorT1;
ω2 = 267.513 * 10^-9 * factorT2; (* for H = 1T, in femtoseconds^-1 *)

J00DipInter = ∫_0^∞ Fitcoef00DipInter[x] Cos[ω1 * x] dx

J11DipInter = ∫_0^∞ Fitcoef11DipInter[x] Cos[ω1 * x] dx

J22DipInter = ∫_0^∞ Fitcoef22DipInter[x] Cos[ω1 * x] dx
```

```
6.15178
```

```
0.956143
```

```
3.89732
```

```
J00DipInter0 = ∫_0^∞ Fitcoef00DipInter[x] dx

J11DipInter0 = ∫_0^∞ Fitcoef11DipInter[x] dx

J22DipInter0 = ∫_0^∞ Fitcoef22DipInter[x] dx
```

```
6.1521
```

```
0.956191
```

```
3.89753
```

```
J00DipIntra = ∫_0^∞ Fitcoef00DipIntra[x] Cos[ω2 * x] dx

J11DipIntra = ∫_0^∞ Fitcoef11DipIntra[x] Cos[ω2 * x] dx

J22DipIntra = ∫_0^∞ Fitcoef22DipIntra[x] Cos[ω2 * x] dx
```

```
2.74046
```

```
0.585208
```

```
2.26827
```

```
J00DipIntra0 = ∫_0^∞ Fitcoef00DipIntra[x] dx

J11DipIntra0 = ∫_0^∞ Fitcoef11DipIntra[x] dx

J22DipIntra0 = ∫_0^∞ Fitcoef22DipIntra[x] dx
```

```
2.74046
```

```
0.585208
```

```
2.26827
```

Calculation of relaxation times T1, T2 (cgs)

```
h = 1.05 * 10^-27; γ = 267.513 * 10^2; factorT1 = 100; factorT2 = 10;
```

$$\Gamma 1 = \frac{9}{8}\,\gamma^4\,h^2\,2\,((J11DipInter0 + J22DipInter0)\,factorT1 + (J11DipIntra0 + J22DipIntra0)\,factorT2) * 10^{48-15}$$

$$T1 = \frac{1}{\Gamma 1}$$

```
0.652868
```

```
1.5317
```

$$\Gamma 2 = \gamma^4\,h^2\,2 \times \frac{3}{4}\left(\left(\frac{3}{8}\,J00DipInter0 + \frac{15}{4}\,J11DipInter0 + \frac{3}{8}\,J22DipInter0\right)factorT1 + \left(\frac{3}{8}\,J00DipIntra0 + \frac{15}{4}\,J11DipIntra0 + \frac{3}{8}\,J22DipIntra0\right)factorT2\right) * 10^{48-15}$$

$$\frac{1}{\Gamma 2}$$

```
0.657357
```

```
1.52124
```

Calculation of relaxation times T1, T2 (SI)

```
h = 1.05 * 10^-34; μ = 4 π * 10^-7; γ = 267.513 * 10^6;
```

$$\Gamma 1 = \frac{9}{8}\left(\frac{\mu}{4\,\pi}\right)^2\gamma^4\,h^2\,2\,((J11DipInter0 + J22DipInter0) * factorT1 + (J11DipIntra0 + J22DipIntra0) * factorT2) * 10^{60-15}$$

$$T1 = \frac{1}{\Gamma 1}$$

```
0.652868
```

```
1.5317
```

$$\Gamma 2 = \frac{3}{4}\left(\frac{\mu}{4\,\pi}\right)^2\gamma^4\,h^2\,2\left(\left(\frac{3}{8}\,J00DipInter0 + \frac{15}{4}\,J11DipInter0 + \frac{3}{8}\,J22DipInter0\right) * factorT1 + \left(\frac{3}{8}\,J00DipIntra0 + \frac{15}{4}\,J11DipIntra0 + \frac{3}{8}\,J22DipIntra0\right) * factorT2\right) * 10^{60-15}$$

$$T2 = \frac{1}{\Gamma 2}$$

```
0.657357
```

```
1.52124
```

Ratio of intermolecular over intramolecular contributions to T1, T2

```
R1 = (J11DipInter0 + J22DipInter0) factorT1 / ((J11DipIntra0 + J22DipIntra0) factorT2)
R2 = (3 / 8 J00DipInter0 + 15 / 4 J11DipInter0 + 3 / 8 J22DipInter0)
   factorT1 / ((3 / 8 J00DipIntra0 + 15 / 4 J11DipIntra0 + 3 / 8 J22DipIntra0) factorT2)
```

```
17.0098
```

```
18.0572
```