Notes
LS2102
Diffusion in Biology

Refer to the Class Recording for Discussion Details

LS2102 (Autumn 2020)

IISER Kolkata

17-11-20

19-11-20

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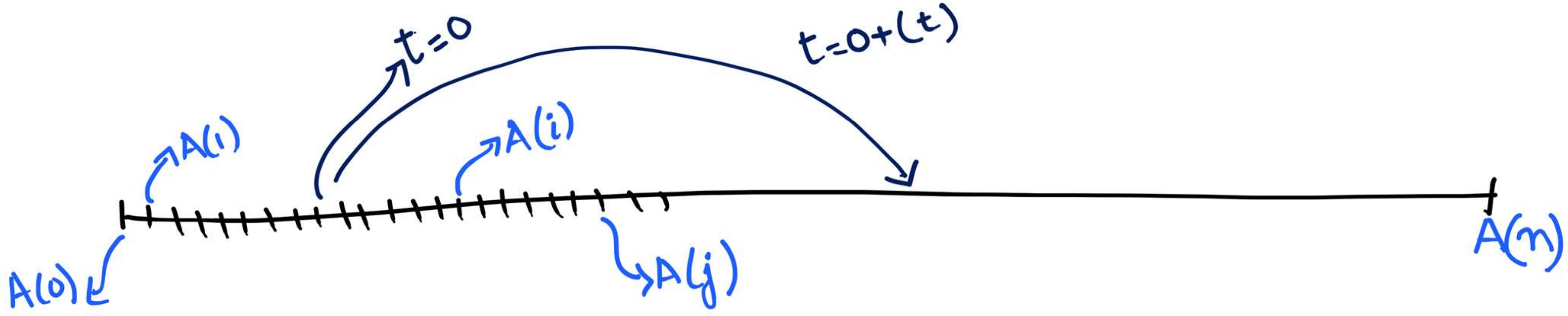
Thursday, 12 November 2020 5:37 PM

TIME CORRELATION FUNCTION : MOVIN- TIME ORIGIN



$$TCF(t) = \left\langle A(0) \otimes A(t) \right\rangle \rightarrow$$

(Arbitrary time origin)

AVERAGE :

1) Over multiple time origins
2) Over many particles

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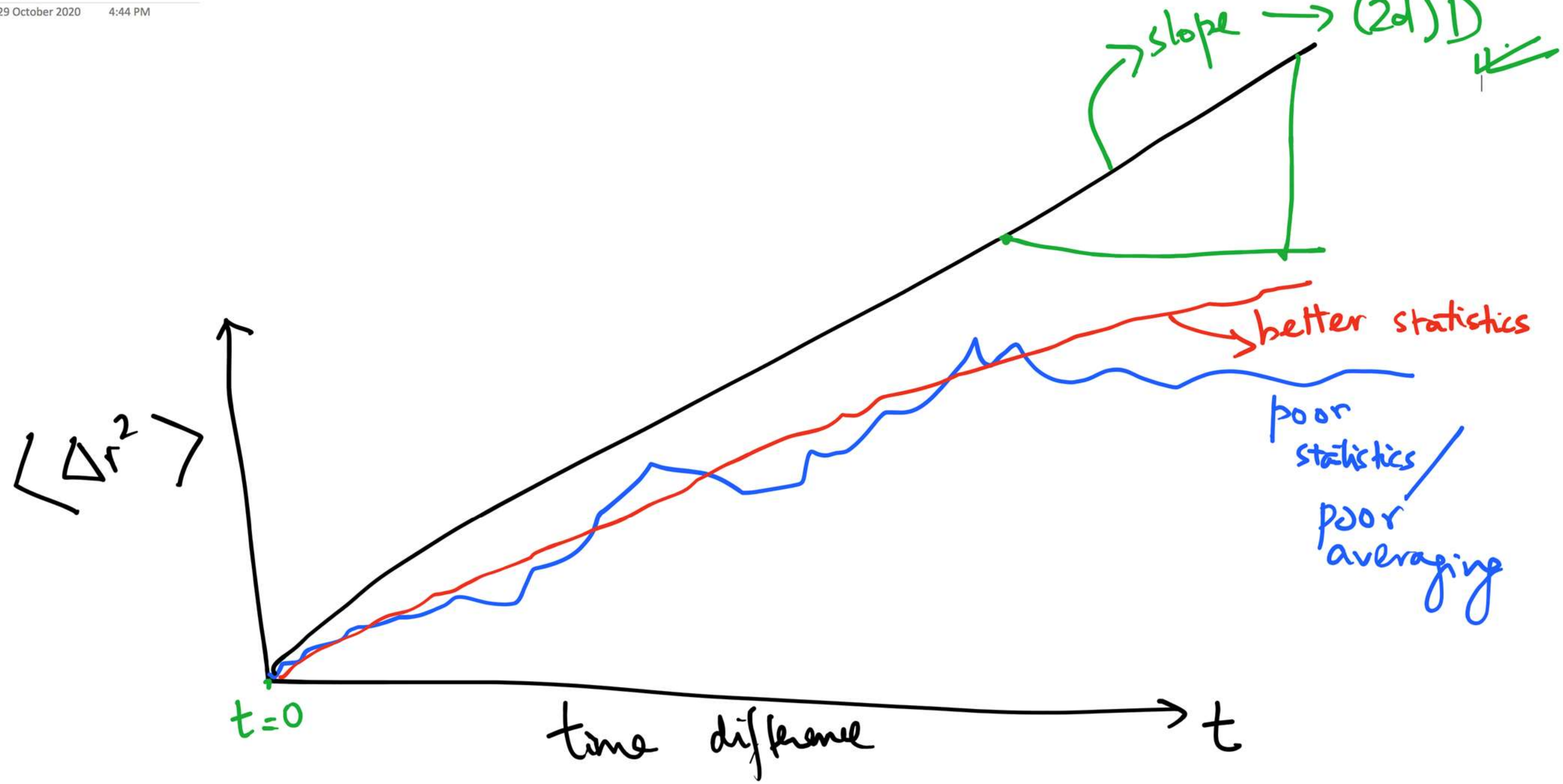

$$\langle \Delta r^2(t) \rangle \equiv \langle\langle |\vec{r}(t) - \vec{r}(0)|^2 \rangle\rangle_1^2$$

→ Average over:

1) Multiple time origins
2) Multiple particles

$$\Delta t = t_j - t_i$$

Format for data file:

m1 $x_0^{(1)}\ y_0^{(1)}\ z_0^{(1)}\}\ \{x_1\ y_1\ z_1\} \dots \{x_{7999}\ y_{7999}\ z_{79}$

m2

⋮

m30 $\{x_0^{(30)}\ y_0^{(30)}\ z_0^{(30)}\} \dots$

A(i)

A(n)

$\Delta t \to n$ → much smaller no. of data pairs

$\Delta t = 0$ → how many time origins → n

$\Delta t \to \frac{n}{2}$ → smaller no. of data pairs.

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$$TCF(t) \equiv \langle A(0) \otimes A(t) \rangle$$

General rule: Your correlation time should be not more than $\sim (1/5)^{th}$ the time points you have from your experiment/computation

8000 data points

- 800 → tcor

→ 1600 → tcor

→

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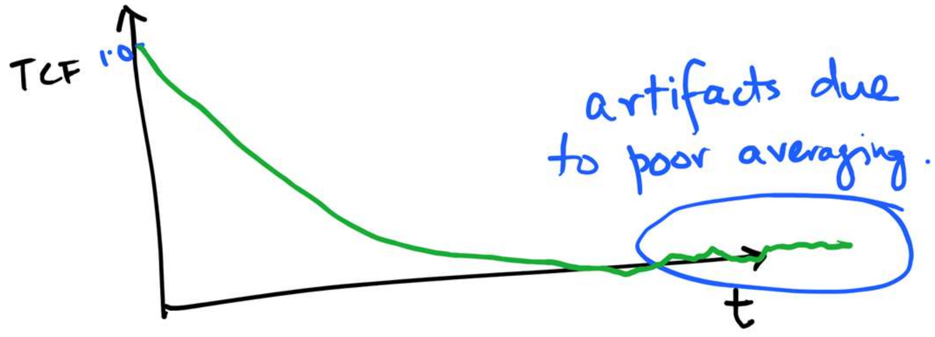

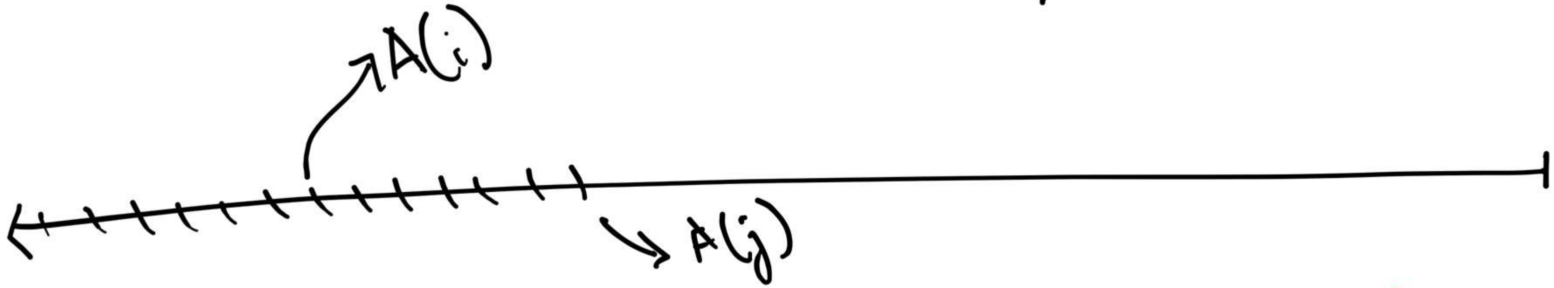

Discrete data points along time

arbitrary arbitrary.

$$\Delta t \equiv \underbrace{t_j - t_i}_{\text{(data pair)}}$$

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Stokes-Einstein Reln.

$$6\pi \underset{=}{\eta} \underset{=}{a} \underset{=}{D} = k_B T$$

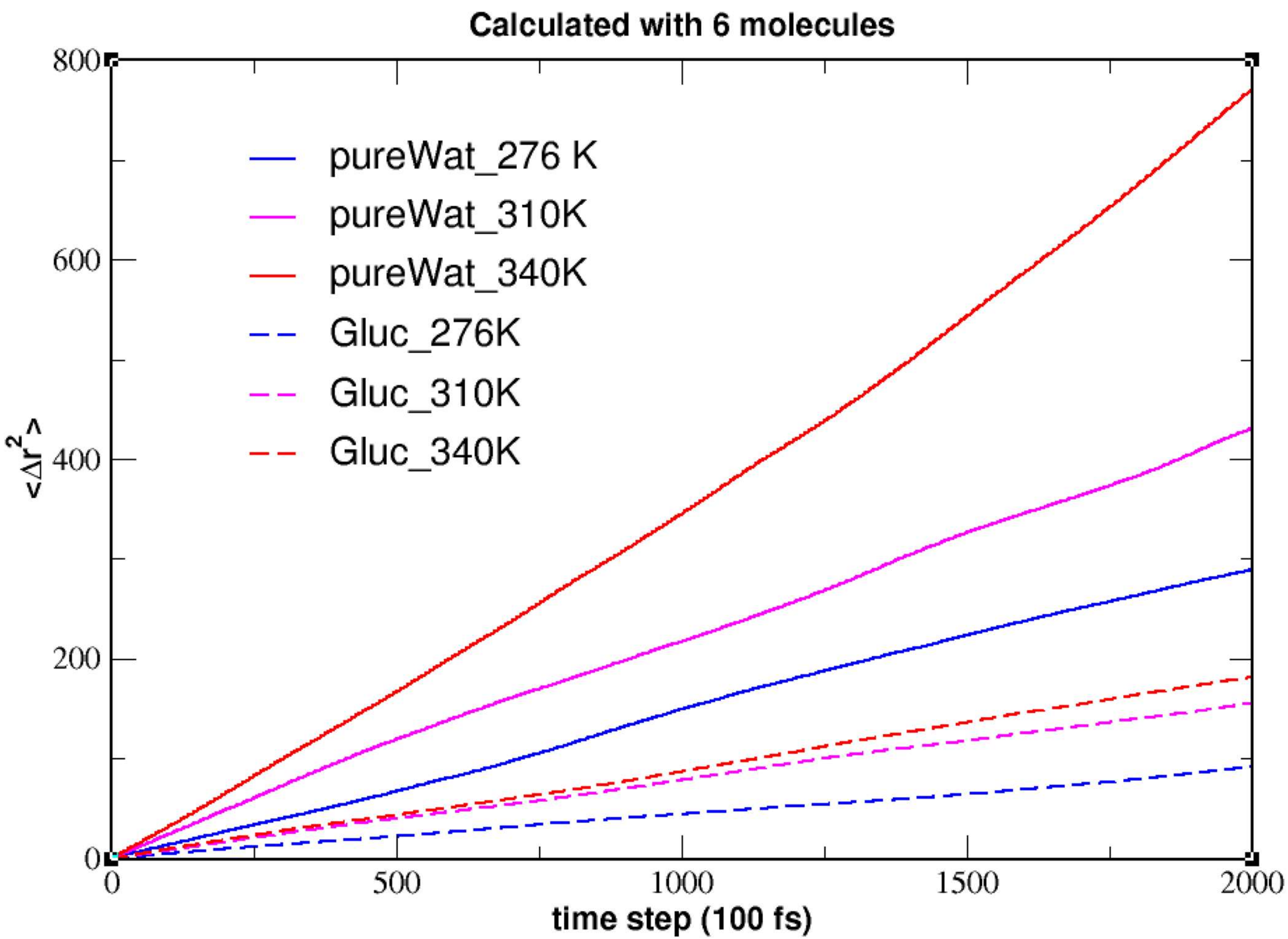
$$a_{H_2O} \approx 5.5 \text{ Å}$$

$$a_{Glu} \approx 30 \text{ Å}$$

At a given temperature (T)

$$\frac{(\eta_{Glu}\, a_{Glu})}{(\eta_{H_2O}\, a_{H_2O})} = \frac{D_{H_2O}}{D_{Glu}}$$

$$\frac{\eta_{Glu}}{\underset{=}{\eta_{H_2O}}}$$



Calculated with 6 molecules
pureWat_276 K
pureWat_310K
pureWat_340K
Gluc_276K
Gluc_310K
Gluc_340K
<Δr2>
time step (100 fs)
0
200
400
600
800
0
500
1000
1500
2000