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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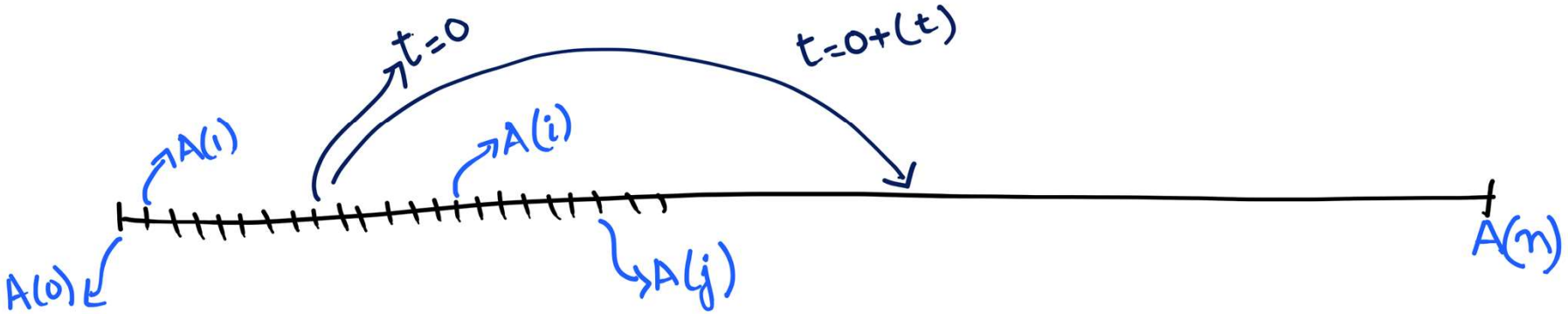
TIME CORRELATION FUNCTION : MOVING TIME ORIGIN



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

(Arbitrary time origin)

AVERAGE :

1) Over multiple time origins

2) Over many particles

8

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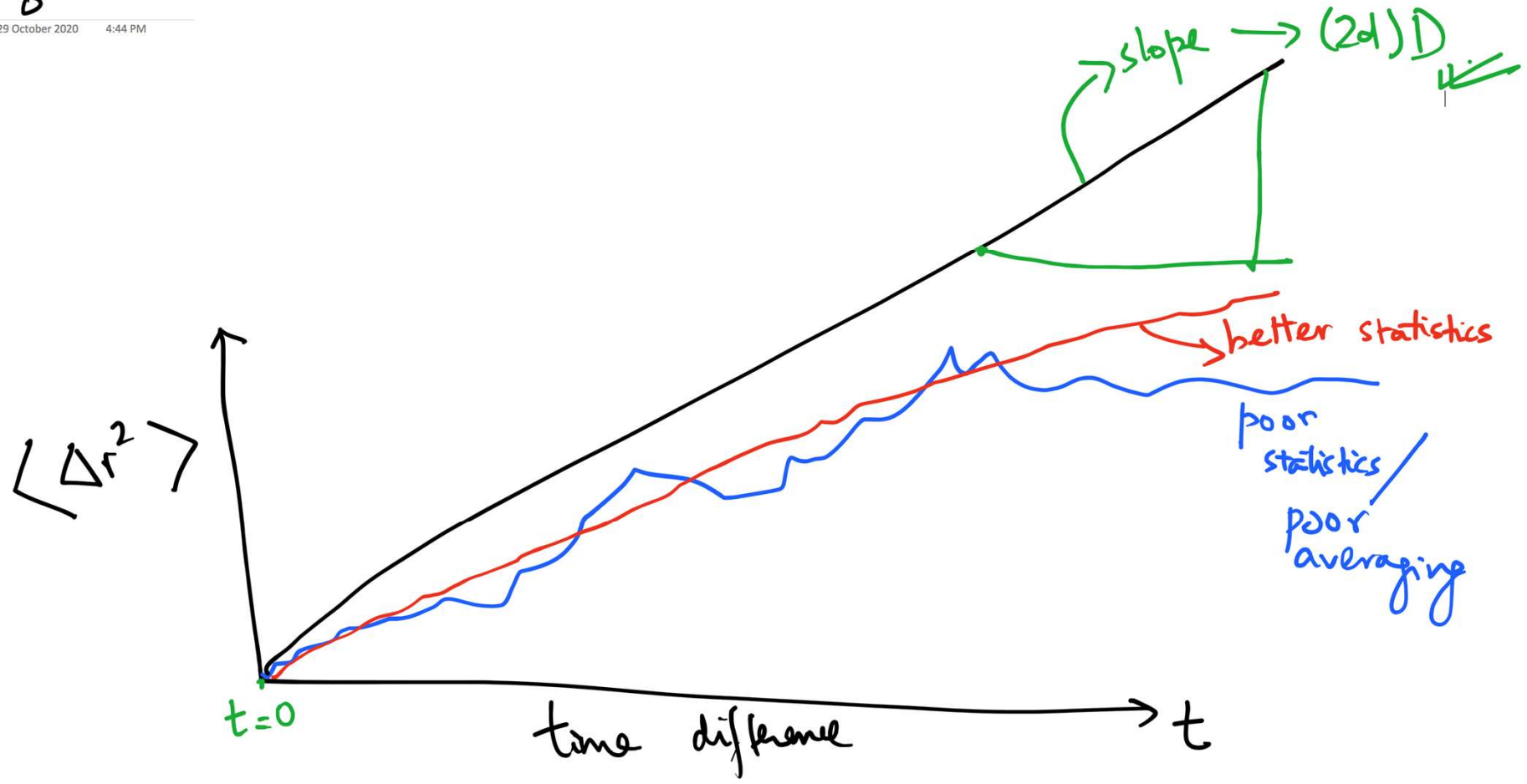

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$$\langle \Delta r^2(t) \rangle \equiv \left\langle\!\left\langle \left| \vec{r}(t) - \vec{r}(0) \right|^2 \right\rangle\!\right\rangle^2$$

Average over:

1) Multiple time origins

2) Multiple particles

$\Delta t = t_j - t_i$

Format for data file:

$m=1$ $x_0^{(1)}\ y_0^{(1)}\ z_0^{(1)}\}\ \{x_1\ y_1\ z_1\}$ . . . . . $\{x_{naaa}\ y_{naaa}\ z_{naa}\}$

$m=2$

$\rightarrow A(n)$

$A(i)$

$m=30$ $\{x_0^{(30)}\ y_0^{(30)}\ z_0^{(30)}\}$ . . . .

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

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

$\Delta t \rightarrow \frac{n}{2} \rightarrow$ 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

800 data points

- 800 → 160
- → 1600 → 320
- →

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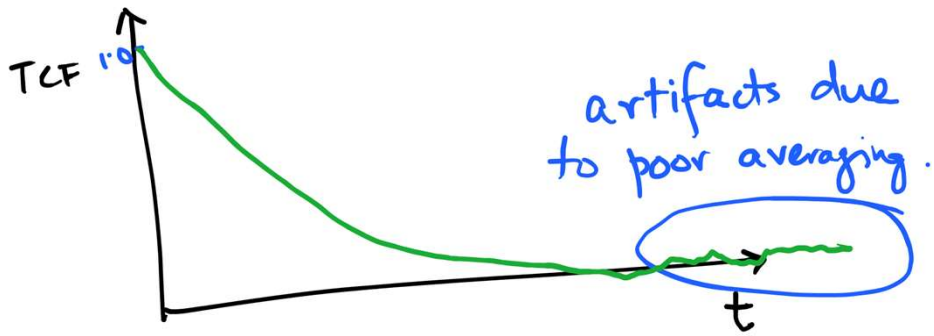
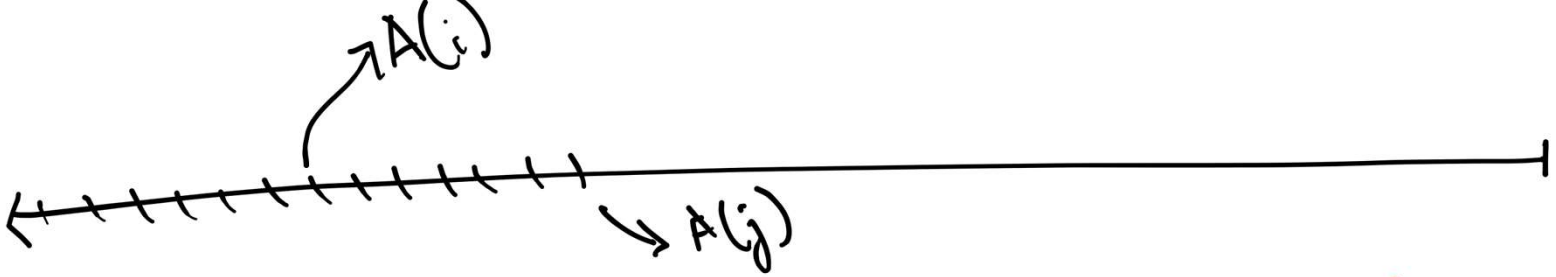




Discrete data points along time

$$\Delta t \equiv t_j - t_i$$

arbitrary

arbitrary

(data pair)

Stokes-Einstein Relⁿ:

$$6\pi\eta a D = k_B T$$

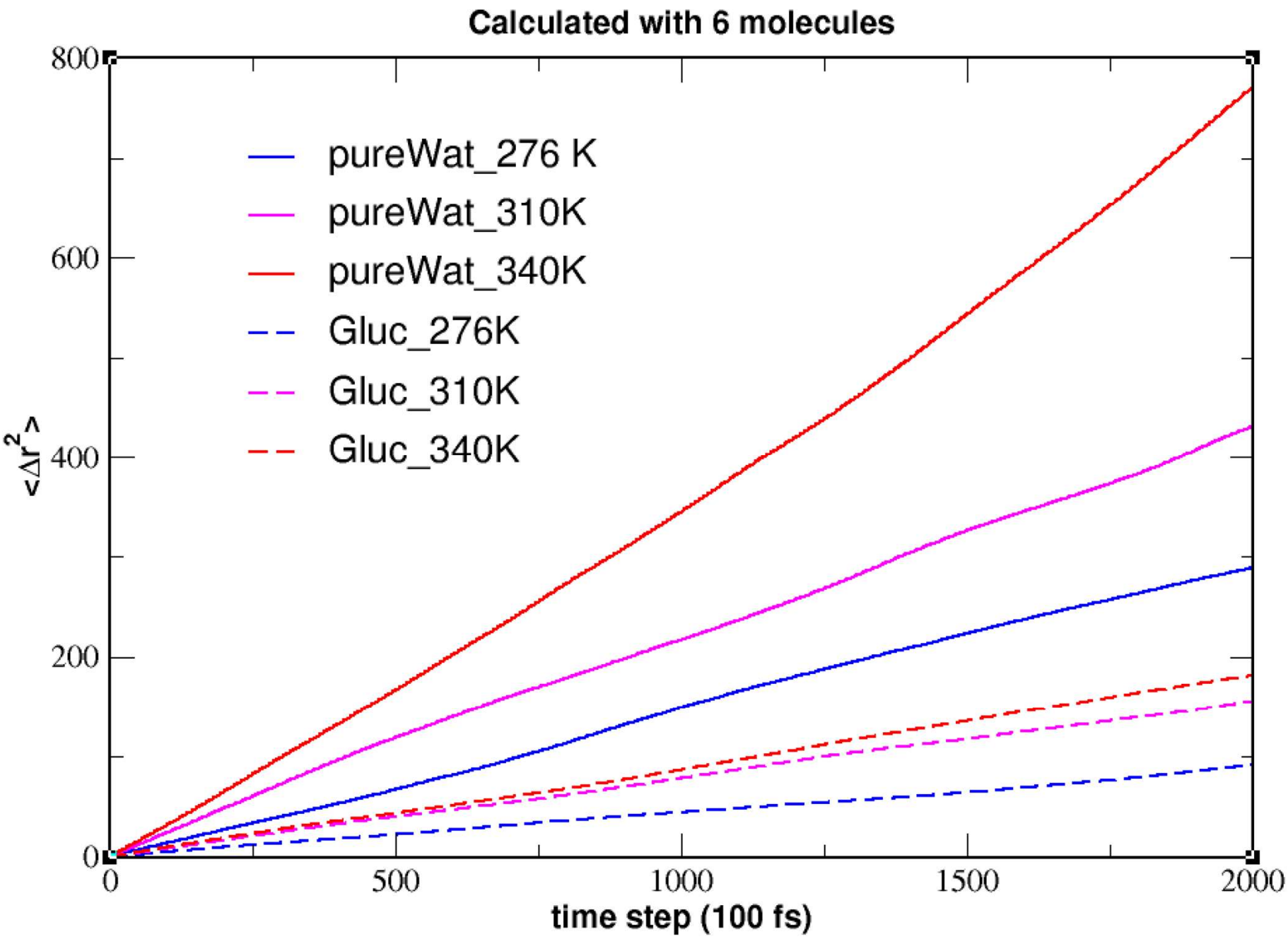
$a_{H_2O} \approx 5.5\,\text{Å}$

$a_{Glu} \approx 30\,\text{Å}$

At a given temperature (T)

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

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


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