

Temperature and Pressure Equilibration

Spoken Tutorial Project

<https://spoken-tutorial.org>

National Mission on Education through ICT

<http://sakshat.ac.in>

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Learning Objectives



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► Ensemble properties



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- ▶ **Ensemble properties**
- ▶ **NVT and temperature equilibration**



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- ▶ **Plot the temperature fluctuation to check for equilibration**



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► Ubuntu Linux v20.04 OS



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- ▶ **Grace v5.1.25**
- ▶ **QtGrace v0.2.6 fork for Windows**



Pre-requisites



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To follow this tutorial,



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- ▶ **Learner must be familiar with basics of Gromacs and VMD**



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To follow this tutorial,

- ▶ Learner must be familiar with basics of **Gromacs** and **VMD**
- ▶ For pre-requisite tutorials please visit this site

<https://www.spoken-tutorial.org>



Code Files



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- ▶ The files used in this tutorial are provided in the **Code files** link



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- ▶ Please download and extract the files



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- ▶ Please download and extract the files
- ▶ Make a copy and then use them while practising



Pressure and Temperature



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- ▶ **Pressure and temperature of the system,**



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 - ▶ **They fluctuate during the MD run**



Pressure and Temperature

- ▶ **Pressure and temperature of the system,**
 - ▶ Are macroscopic properties
 - ▶ They fluctuate during the MD run
- ▶ They are calculated from the average velocity and position of the ensemble



Pressure and Temperature



Pressure and Temperature

- ▶ Here, ensemble consists of all the particles in the system



Computation Time



Computation Time

- ▶ Having more steps in MD takes longer time



Computation Time

- ▶ **Having more steps in MD takes longer time**
- ▶ **Use a computing facility to run these processes**



Computation Time

- ▶ Having more steps in MD takes longer time
- ▶ Use a computing facility to run these processes
- ▶ Take care not to overheat or burn your computer



Summary

- ▶ Ensemble properties & equilibration
- ▶ Performed **NVT** and temperature equilibration
- ▶ Plotted the temperature fluctuation and checked for equilibration
- ▶ **NPT** and pressure equilibration
- ▶ Plotted the pressure fluctuation



Assignment



Assignment

- ▶ Plot density and volume of the system after `NVT` and `NPT` steps
- ▶ Recap processes and commands starting from `1AKI.pdb` to equilibration
- ▶ Read publications of your choice using `Gromacs`



Assignment



Assignment

- ▶ Open the `nvt.gro` and `npt.gro` files in `VMD`
- ▶ Ascertain that, protein is not seen as two parts on two sides of the box



About the Spoken Tutorial Project

- ▶ Watch the video available at https://spoken-tutorial.org/What_is_a_Spoken_Tutorial
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Spoken Tutorial Workshops

The Spoken Tutorial Project Team

- ▶ Conducts workshops using spoken tutorials
- ▶ Gives certificates to those who pass an online test
- ▶ For more details, please write to contact@spoken-tutorial.org



Forum questions

- ▶ Questions in THIS Spoken Tutorial?
- ▶ Visit <https://forums.spoken-tutorial.org>
- ▶ Choose the minute and second where you have the question
- ▶ Explain your question briefly
- ▶ The Spoken Tutorial project will ensure an answer

You will have to register to ask questions



Acknowledgements

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