Thermodynamics for Biological Systems:
Classical and Statistical Aspects
Prof. Sanjib Senapati
Department of Biotechnology
Indian institute of Technology - Madras

Lecture – 76
Link between Theory and Experiment

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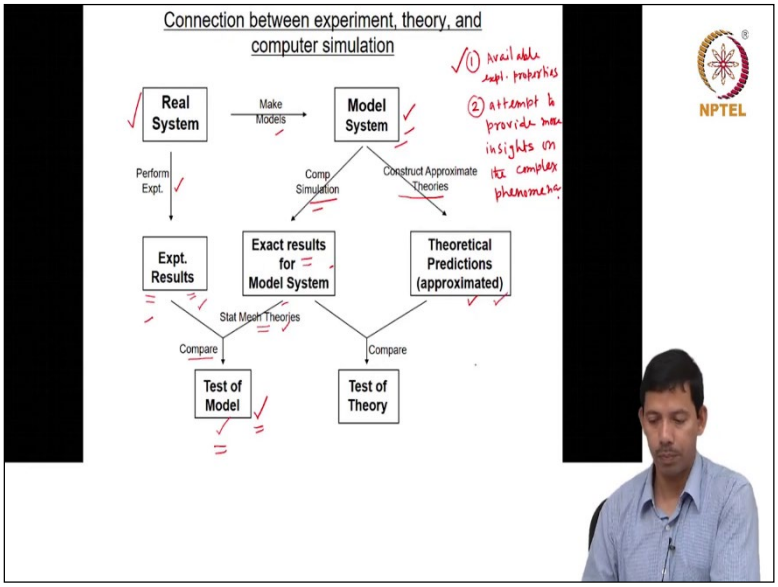

So, how we can make a connection if we do a computer simulation, how can we make a connection of the simulation results, how do we trust the simulation results and this is the link what computer simulation simulator mix with the experimental data. So, let us say we have a real system here so this real system could be biological system or it could be on liquid system or anything of your interest. So, you start from this real system and starting from this real system you make a model this is very important.

You make a model you make a basically you make a model to obtain a model system. So, what do you mean by making a model? As I said that you make a model of water by describing that it has hydrogen oxygen hydrogen it has HO bond it has OH bond it has a HOH angle and it has partial negative charge and oxygen and partial positive charge on that two Hydrogen, so you make the model and that is your model system.

Once you have the model system you can perform computer simulation on your model system. Once you far from the computer simulation you get the results so those are the results you obtain from computer simulation for the model system you have made. On the other hand from real

system you perform experiment and you get the experimental results. So, experimental results are the accurate results what you get from experiments.

And in this side you got the results from your model system by carrying out a computer simulation now what you do you basically okay. Now you apply statistical mechanical theory from your computer simulation data and using the statistical mechanical theories you get you generate the same thermodynamic quantity for which you have the experimental data. Now you compare your experimental data with data you often from computer simulation and statistical mechanical theories.

And if they compare very well then you can say with confidence that my model system was very good. If your results do not match then you need to go back here and remake your models so then your model was not good and so your model needs to be remained so you remake your model. So, remake your model make a new system for from computer simulation get the data apply statistical mechanical theories to obtain the experimentally known thermodynamic quantities match them and now if they compare very well so you know that your model system is pretty good.

So that is how you basically make sure that your computer simulation method was robust. So, once you get a good match of the quantities for experimental data are available so you know that my simulation protocol and my models are good. So, once you get that confidence that my computer simulation was good so you can further go deep inside and obtain more information of the system reach where other difficult to obtain experimentally.

In other words what I try to say is that first you match your simulation data with available experimental with available experimental properties, with available experimental properties once you see that they are matching pretty well, so in the next step you can attempt you can attempt to provide more insights on the so on that complex systems for which on the complex system or phenomena which were difficult to obtain experimentally.

So that is the robustness of complex incessant technique so in compressible simulation technique to some extent also make a bridge between the experiment and theory in a sense that once you make the model and you see that your model is doing pretty good by matching with external data you can also construct approximate theories on the model system. And from there you get the

theoretical predictions and if you now compare your theoretical predictions with the exact result from computer simulation so that is our test of theory so it is said that in a sense computer simulation makes a bridge between the experiment and the theory.