

Re: state variables

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 - *Date:* Sat, 22 Oct 2005 16:47:02 +0000 (UTC)
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When talking about proteins and their interactions, it's important to mention on what scale you're aiming to model them. Individual proteins are huge (thousands of daltons), have several different stereochemical forms, and hence different electrical, polar, and bonding site behaviours based upon their current configuration.

Some physical chemists make a study of looking at a single type of protein at small scale and developing thermodynamic models for the changes in shape from one conformation to the next.

At a higher level, molecular biology people are less interested in this than the reaction rates of a population of said protein or, more often, a soup of various proteins that represent part of a biochemical pathway. For this type of model, the different conformations of a protein might be modeled as different populations such that P1a (protein 1 in configuration a) is tracked separately from P1b (protein 1 in configuration b), etc., with some probability over time of P1a turning into P1B (or vice-versa) due to a configuration change, or other control.

This all relates to computer modeling of the situation. I usually work from the target to the mathematical model to the simulation. My first question for you, in creating a thermodynamically valid approach, would be to ask you at what level you want to simulate or mathematically model this system.

I'm not sure if this helps at all. But if it does, great!

–Munir

P.S. Check out the ERATO simulator at Caltech if you need a good database and simulation system without starting from scratch.

P.P.S. The above discussion of different state variables being thermodynamically complementary to each other is informative. Thanks for a good and useful thread.

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- **References:**

- ◆ **state variables**
 - ◇ *From:* biplabbose
- ◆ **Re: state variables**
 - ◇ *From:* Igor Khavkine
- ◆ **Re: state variables**
 - ◇ *From:* Arnold Neumaier
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