IKT in TKJ4215 – Statistical Thermodynamics in Chemistry and Biology

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The course

TKJ4215 – Statistical Thermodynamics in Chemistry and Biology is an obligatory course for the nanotechnology students (MTNANO) on the 2nd year in the spring semester. It is also optional for the chemical engineering students (MTKJ) and the chemistry students (BKJ/MSCHEM) primarily on the 3rd or 4th year of the studies. The course is taught in English since 2-3 exchange students are accepted every year. Normally, the course is followed by 30-40 students.

The course gives an introduction to statistical thermodynamics with a chemical perspective and thereby also to classical thermodynamics. For example it introduces entropy through Boltzmann's law, partition functions and Boltzmann's distribution law. Lattice models are used extensively to provide simple models for estimating the multiplicity (and thereby the entropy) through basic combinatorics (multinomial distributions).

The course is organized with regular lectures (4 hours per week) and voluntary "pen-and-paper" exercises (4 hours per week) where standard problems are solved. There are no laboratory exercises.

New computer-based exercises

In many parts of the course, approximations are introduced so that the problems can be solved by "pen-and-paper". By just avoiding a few approximations in some cases, the course would be ideal for solving exercises by basic numerical methods. By introducing computer-based exercises, the relevance of the course would be increased by solving more realistic problems as well as that numerical methods would be introduced/used in a natural context.

Python will be used and examples of tools that will be used on relevant problems include:

- Using numpy and scipy to solve a linear system of differential equations (e.g. in kinetics).
- Using numpy and scipy for numerical integration.
- Using sympy for symbolic mathematics (mainly differentiation and integration).
- Using matplotlib for presentation of data (mainly two-dimensional graphs).

The first example, using linear algebra, is the main type of exercises that will be introduced. More possibilities exist, but their feasibility need to be investigated as a part of the project.

The goal is to develop 10 exercises where one exercise is supposed to be solved in a 2-hour exercise session. After a pilot year when the course is given in the spring 2016, it is expected that these exercises will be compulsory from 2017. The exercises can be solved either in a computer room or on the student's own computer.

Application

We apply for 150.000 NOK, which will be used for a part of the duty work for a Ph.D. student, Oda Dahlen. She has a background as a nanotechnology student (and has therefore taken the course) and is now a Ph.D. student in theoretical chemistry. She is therefore an ideal person to carry out the work. She will use 12 weeks (450 hours) on the task divided into using 8 weeks (300 hours) in 2015 to develop the exercises and 4 weeks (150 hours) during and after the course in 2016 to evaluate (including writing a brief report) and improve the exercises.

An own contribution from the Department of Chemistry is provided in terms of 50 hours for Prof. Per-Olof Åstrand. He will coordinate the project and provide suggestions for suitable exercises. He will also adapt the lectures and the remaining part of the exercises so that the computer-based exercises become a natural part of the course.