Teaching Molecular Dynamics for MST engineers

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http://www.imtek.uni-freiburg.de/simulation/

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A short version has been published in MST News, International Newsletter on Microsystems and MEMS, 2003, pp. 34-35.

Conventional continuum-level modeling based on finite element method may become inadequate to treat nano-objects. Hence, a microsystem technology (MST) engineer should be aware of an alternative approach, that is, molecular simulation, because MST becomes MNT (micro- and nanotechnology).

This happens not to be an easy goal because an engineer does not have much experience with molecule-oriented problems. On the other hand, molecular simulation software has flourished over the last ten years and many free and commercial software packages are available on the market. In principle, this allows an engineer to employ this software at the user level to solve a particular problem but the main problem is a lack of general knowledge in this area.

The course Molecular Dynamics for MST has been created at IMTEK three years ago. The main emphasis during the course is made on the ideas rather than on mathematics. A student by the end of the course should be able:

- to understand the results of research in molecular simulation;
- to decide when molecular simulation is more applicable than a conventional finite-element simulation;
- to choose on what level to describe a potential energy surface (ab initio quantum chemistry, semi-empirical quantum chemistry, or molecular mechanics);
- to select an appropriate molecular simulation in order to obtain the desired result;
- to understand the input parameters compulsory for the simulation;
- to roughly estimate the simulation computational time.

The course is accompanied by small computational labs: molecular dynamics with the in-house developed software, quantum chemistry with GAMESS, and visualization of proteins with Swiss-PDB Viewer.

Below we briefly describe the course syllabus.

1) Introduction (1 lecture)

   We start the course by giving a few examples of molecular-level applications in order fascinate students and then present the Big Picture of molecular simulation.

2) Particle dynamics (3 lectures)

   In order to make molecular simulation more concrete for a student, we decided to start with molecular dynamics of particles. Our students know theoretical mechanics well and it is relatively easy to explain them the main idea of molecular dynamics with an example of a fluid consisting from atoms/particles. We consider here how to integrate the equation of motion of interacting particles, compute the forces between all particles efficiently and process particle trajectories in order to extract useful information.

3) Statistical Mechanics (1 lecture)

   As post-processing of particle trajectories is based on statistical mechanics, we review its basis. The Monte-Carlo method is introduced as an alternative to molecular dynamics and their advantages and disadvantages are discussed.

4) Potential Surface Energy (3 lectures)

After the students have understood how one can run molecular dynamics or Monte-Carlo simulation, they are asked where one can find an expression for the potential energy. Then we consider possible answers, that is, the quantum chemistry and molecular mechanics (empirical force field). Here the goal is to introduce students to basic ideas and learn the most important abbreviations he/she can encounter in practice. At the end, we consider a problem of how to search for the global minimum on the potential surface energy with an example of protein folding.

5) Advanced molecular simulation (2 lectures)

After a student obtained basics understanding of how one can use molecular simulation to obtain useful engineering information, we concentrate on how to compute the answer for the given limited computational resources. To this end, we consider how one can reorganize the simulation in order to compute the phase equilibria and rate constants efficiently. At the end, multiscale simulations are reviewed when one splits the computational domain to several zones in order to combine different level of theories (for example, molecular dynamics and finite element analysis) together.

6) Empirical Correlations (1 lecture)

Molecular simulation is computationally demanding. As a result, the empirical method Quantitative Property - Structure Relationship enjoys widespread use among practitioners. We decided to devote it the final lecture of our course and stress once more that an engineer must be pragmatic. If some approach requires too much computational power today, one can always find a simpler way to achieve the practical goal.

In order to check whether the chosen structure allow us to achieve the course goals, we assigned research scientific papers on molecular simulation related to MNT research (for example, organic electronics) to students. They should present the assigned paper at the end of the course as if it were made by themselves. We have found that the most students were quite successful with this: they were able to understand what has been done, what is of importance to MNT engineers, and why it has been done this way. As a result, we believe that our course is a good way for MST engineers to understand what the molecular simulation community is doing.