Ontology design for physical chemical systems

Heinz A Preisig NTNU - Trondheim, Norway heinz.preisig@chemeng.ntnu.no

Background

Computational engineering is getting more and more a central activity in all engineering disciplines. It certainly will also increasingly affect chemical engineering as the trend is towards multi-scale computations in particular simulation covering the full range: quantum and nano scale ab initio, micro scale and meso-scale structures, as well as macroscopic design and operation-related computations. This requires a shift in education and specifically a shift towards more computation related education as well as a widening of the knowledge base that chemical engineers take along from their education.

On the research side we increasingly see an integration of material-related computational activities with traditional chemical engineering computation tools. Specifically large-scale optimisation has been applied to the particulate domain, which intrinsically is a very large-scale energy minimisation problem. Otherwise, many of the associated techniques, such as computational fluid mechanics, ab initio computations, micro and meso-structure computations have not really made the impact on the profession than one would expect.

Whilst one will focus on continuously improving the computational capabilities by designing new and improved algorithms, programs and work on implementing workflows across the tools and scales, one should also observe a refocus of a large group of users towards the structures of the problem they work on in contrast to developing algorithms. This will increase the productivity of the engineers in particular the quality of the work will increase whilst the required time will decrease. The change will really only going to happen in a larger scale if one succeeds to have more people have a broad knowledge and if the providers construct a computational frame work, that is easy to use and constructed around consistenat basic information. To mention an example it should not be the case that one constructs and performs simulations that do not close the basic conservation principles.

Presentation

Besides the background, I will discuss a structure for an ontology suitable for the represenation of physical-chemical-biological systems. The structure is buidling systematically from a starting piece of information, namely a directed graph consisting of nodes and arcs. Information is added each time defining a new piece based on what has been defined before. Thus the information is build in a lower triangular form, or what in compiler construction is called a context-free definition.

One or two example will be used to explain the use of the ontology: a reactive flash and a stirred tank reactor with feed, some outlets and a breathing pipe, with a three phase system in the contents, an extractive reactor.

These two systems have most of the components one would normally find in the processing industry.

Comment Could also fit into 10E00 or 10E04