Mismatch Between Simulation and Experiment? Let's Consider Model Systems for Better Interplay!

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Do we agree that, as results of the promulgation of computers and progress in computer science and computational theory made in the last couple of decades, there are ample examples of successful application and utilization of simulation technology today? If we consider product-oriented simulation technology such as computer-aided design (CAD), we may have the impression that such technology is well past the evaluation phase and has already become ubiquitous. If we think of material-oriented simulation technology, however, successful cases may seem to be few in number.

Simulation technology is used in two phases: analysis and design. The former starts with a validation of the methods and models employed. The simulation results are validated against the phenomena or properties measured to ascertain that the target attributes and features are simulated precisely. This is a vital process for any system. Unfavorable results obtained in this process will not allow the researcher to move to the subsequent process of identifying dominant factors, let alone the design phase that follows. In this case, the reputation of simulation technology may be considerably harmed.

What is important for the validation of a simulation? Naturally, there may be a variety of factors that are case-dependent, but for the purpose of simplification, let's take instrumental analysis as an analogy. The measurement results can only originate from the sample used. Therefore, after determining the measuring instrument, it is the sample preparation that determines the spectra that will be obtained. Ideally, the samples of practical structure should be measured in operando, i.e., in an actual operating environment. We have to, however, use model measurement method due to constraints such as a sample holder in many cases. High-precision measurement is also desired, for example, using SPring-8 (large synchrotron radiation facility). However, we are often obliged to perform measurement with devices readily accessible from a laboratory on a daily basis even if less accurate. Similar issues arise in terms of selecting simulation methods and a computational environment. Simulation results are fully determined by the parameters and structural models as an input once the methods are chosen. If there is a discrepancy between the simulation results and actual measurements, it must be attributed to the accuracy of the parameters of physical properties or structural models that are employed, supposing that the methods and computational conditions are appropriate. It is not difficult to assume that, in molecular simulation, presupposition of an ideal composition or surface/interface structure causes the discrepancy. In finite element analysis, a discrepancy may be attributed to the simplified representations of complex structures, such as a porous structure, and the use of encompassing values as physical properties. When researchers and engineers come across such a discrepancy, how would they respond?

For instance, some may opt for an alternative approach assuming that the simulation technology is not likely to help. Others may make effort to tune the simulation so that the results agree with the actual measurements. Is it too much to say that these actions are a 20th century approach? One may consider that the measured object must be different from what they have assumed and try to measure again after a careful consideration of conditions. It is too idealistic, conversely, if I call it a 21st century approach. What is the reality in laboratories of today? Rather than considering the current status, we should foresee the situation in 15 years' time, around the year 2030, to see the ideal conditions for addressing the issue. It is envisaged that the population of Japan will decrease by 10 million, with a higher proportion of elderly citizens. While China has gone into a population decline, that of India is still growing, and it will have surpassed China. Given this trend, to maintain a global competitiveness, Japan must consider deploying intelligence in manufacturing, although it has hitherto largely relied on spirit, intuition and guts. Simulation technology is a tool to facilitate virtual experiments using models that represent the reality, leveraging the human "knowledge" implemented as software on a computer. Even if a computer works over 8,000 hours per year, it won't raise the issue of unethical labor conditions, nor will the supervisory authority intervene in the issue. Looking at society in 15 years' time, what can we do to ensure the younger generation, who will be the driving force of their companies, can be at ease with using

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simulation technology?

The young researchers and engineers who are already adept at using simulation technology today will be assuming positions as leaders or assessors in 2030. They will have appropriate evaluation standards in place, as well as the competence to practice them. Then they will need to focus more on the training of those who follow. Imagine a future where we have more young talents who can support better 'interplay' between experiments and simulations. When they come across discrepancies between them, they may intend to propose that they should experimentally measure the sample characteristics to validate the simulation based on an ideal model experimental system, in addition to conducting the simulation based on a realistic system model rather than an ideal system model. Such promising researchers or engineers will start to play an active part one after another. If this is the picture of our future, there must be a variety of options that we can look into.

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