Instrument Simulation --Why, What to Expect, What tools to use

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Abstract

At past HEMS conferences, I have spoken about SIMION and our efforts to expand its usefulness, improving accuracy, using it to analyze fields, and applying it to the synthesis of ion optics. This year, I will address broader questions about the utility of simulations as partners in design and experiment.

Over my forty-year career designing scientific instruments, I have seen good reasons for skepticism toward simulations. Sometimes they were too crude, limited by the available software and computing hardware. While expectations were too high, they were high on both the simulators' part and the groups requesting the simulations. In this talk, I will revisit these misgivings, considering greatly improved software and hardware, and I will emphasize the necessary interplay among simulation (i.e., theory), intermediate experiments, and multiple-hypothesis testing—the very bedrock of expedient scientific progress.

Another key consideration today is the advent of powerful artificial intelligence tools. When used judiciously, AI can enable even infrequent users of simulation software to set up and run effective simulations, and to write code that once required deeper expertise.

I will also review recent developments in simulation tools—not only SIMION but also Multiphysics approaches, both commercial and open-source, including COMSOL, OpenFOAM, MEEP, and the MOOSE framework. While no single designer can master all of these, I hope to show that the combination of available tools and AI may usher in a renaissance in scientific instrument simulation and design—bringing models closer to reality and fostering a community of simulation practitioners more tightly integrated with instrument designers.

Finally, I will discuss the use of simple Git commands not only for revision control but also for results documentation, highlighting the workflow I have implemented in SIMION as an example. I look forward to stimulating discussion both during the talk and throughout the conference.

Biography - Bob Jackson

Bob Jackson has a BS in engineering Physics and a master's and Ph.D in Physics. He designed scientific instruments as an undergraduate and graduate student, He was a postdoctoral fellow at the Laboratory for Surface Science and Technology at the University of Maine NSF MRI grant to develop a HREELS Tof. He previously worked as an Electrical Engineer for a high-power RF transmitter company. His career has involve 4 startup scientific instrument companies and work for an Ion Mobility manufacturer.

Keywords

Scientific Instruments, Simulation, Design