After Nabarro

With the passing of Frank Nabarro in July of this year, we have lost one of the founding fathers of materials science. His name appears in many of the textbooks from which we train our students today, and also on the spines of several volumes on dislocation theory, including his classic monograph on the subject. He rightly stands among the gods of our field. Ninety years old at his death, he was a sprightly dancer at the frontiers of knowledge, right up to the end.

Nabarro was an "old school" materials theorist. He used insight to inform mathematical formulation, then used the mathematical results to develop even deeper insight into the strength of solids, especially in the area of dislocation theory. For him, the details of the mathematics never seemed as important as the underlying principles that they revealed, and by applying the principles, he was able to leapfrog others and quickly identify the solutions to new problems. For those who care to look, his book *Theory of Crystal Dislocations* (originally published by the Oxford University Press in 1967, then reprinted by Dover in 1987) presciently contains the answers to many questions that have only just begun to be considered by others, just because he thought the topics provided interesting illustrations of the underlying principles.

But dislocation theory is a complicated subject, and like many such subjects, it has been studied increasingly through the use of computers. Codes are now in use that can track millions of dislocation segments, or even billions of atoms to find the dislocations. These simulation algorithms allow the researcher to observe how dislocations interact, multiply, and organize themselves during plastic deformation, fatigue, and fracture, and to test how changes in the applied stress or other details of the experiment change its outcomes. They are truly remarkable achievements, and the graphical output is seductive and fascinating. It allows us to see things that cannot be seen using any other tool.

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Computer simulation in dislocation theory fits the description of a "disruptive" technology provided by Clayton Christensen of Harvard Business School in his 1997 book, *The Innovator's Dilemma* (Harvard Business School Press). A disruptive technology does the same job as an existing tool (for example, pencil and paper) and eventually completely displaces the existing tool. Christensen notes that most disruptive technologies initially have serious shortcomings compared with the tools they replace, but they provide some advantages for less-demanding users. Images from the first digital cameras, for example, were no match for film, but they were nearly instant and much more easily reproduced; as the technology advanced, propelled by market forces, it has eventually exceeded the capabilities of the older method, and has opened new possibilities, too.

Many of the early results of dislocation theory arising from large-scale computer simulation have been rather trivial, providing answers that could have been derived in five minutes with a pencil and paper (or without the benefit of even those tools, in the mind of Frank Nabarro). In many cases, the computer simulations have produced answers that were wrong, because although they simulated millions or billions of atoms, they failed to take into account some aspect of the physics. In most cases, still, the simulations are limited either in their length scale or their time scale, both of which are vitally important in many problems of dislocation dynamics. Continuum theory does not face these limitations, but does have others.

As the availability of teraflops computing grows, computer simulation is beginning to outpace the capabilities of traditional theory. It can address problems that would be intractable with any other tool, produce data faster than the human mind can absorb it, and present information in attractive visualizations. Somewhere along the line, though, the vital role of a Frank Nabarro seems to have been lost. His great contribution was the ability to make sense of all the theoretical developments. Sometimes it seems that computer simulation results are offered without any thought as to whether they make sense relative to the "traditional" insights produced by Nabarro and others. Almost always, computers lack the ability to synthesize new physical principles from the deluge of data. Being able to simulate is not the same as being able to understand. Perhaps this understanding will come as simulation moves from being the disruptive technology to the dominant tool of dislocation theory.

The mid-20th–century U.S. radical Abbie Hoffman once remarked that the 1960s was such a great decade that it didn't end until 1972. In dislocation theory, the latter half of the 20th century was a golden age, and it didn't bow out until 2006. With Frank Nabarro gone, we now have to reinvent some of its capabilities.

Alex King

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