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LETTERS:

Validating the Need to Validate Code

Douglass Post and Lawrence Votta's article admirably stresses the need for validation of computation. If I understand their main point correctly, it's that computation is science, not mathematics.

The article motivates me to contrast two fields I work between that use very different paradigms to describe the electrodiffusion of charge. In computational electronics,[1,2] the electric field is traditionally calculated by solving Poisson's equation with far-field boundary conditions but at relatively low resolution. Poisson is solved anew whenever charges move. Computational chemistry, starting more or less with computer simulation of fluids[3] and computational biology,[4] computes the electric field at high resolution and does not deal clearly with far-field boundary conditions.

Electrodiffusion, which has been at the center of electro- and physical chemistry since Michael Faraday's time, is also at the center of electronics, where it describes the movement of charge in semiconductors and most of our digital devices. Electrodiffusion is no less important in biophysics, where it is responsible for the electrical properties of cells and tissues, and controls many biological functions.

It seems to me that these different treatments of similar physics are distinct and unlikely to be equally precise under all conditions. I hope the article helps motivate workers in each tradition to discuss other treatments beyond their own and try to understand the differences. I hope such workers can determine the conditions under which each treatment is accurate. That way we may learn to use each computational tradition of electrodiffusion only in appropriate situations.

References

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