TechAndComputer (Nov. 28, 2012) — Picture two charged particles in a vacuum. Thanks to laws of elementary electrostatics, we can easily calculate the force these particles exert upon one another, and therefore predict their movements.

Submerge those particles in a simple medium -- say, water -- and the calculation grows more complex. The charged particles' movements influence the water, which in turn may slow, speed, or otherwise alter the particles' paths. In this environment a prediction must also consider the water's reaction, or its dielectric response.

But in real biological and material systems, media are also complex: plant cells and blood cells, for instance, are made up of several media and may be oddly shaped. This heterogeneity has made predicting the movement of charged particles in complex environments extremely challenging for theoretical physicists.

Now researchers at Northwestern University's McCormick School of Engineering have developed a model that can predict the reactions of charged particles in any media. Their computational discovery, which takes cues from nature, could find applications in biology, medicine, and synthetic materials research.

The model is the culmination of seven years of work by Monica Olvera de la Cruz, Lawyer Taylor Professor of Materials Science and Engineering, Chemistry, and (by courtesy) Chemical and Biological Engineering at the McCormick School of Engineering, with partners from Arizona State University.

Creating molecular simulations in heterogeneous media requires two steps: measuring the effects of the medium's dielectric response on the charged particles and measuring the effects of the charged particles on the medium's dielectric response. In previous attempts at such simulations, models treated the two calculations separately, completing one set of calculations before turning to the next. This process required solving a differential equation that governs the motion of the charged particles -- namely, the Poisson equation -- at each step of the simulation.

The Northwestern researchers have developed a new, faster way that avoids the Poisson equation entirely. Using insight gleamed from nature, they have reframed the electrostatic problem as an energy-minimizing problem.

"Nature doesn't wait to figure out the response of the medium in order to move the charged particles, nor does it wait to position the particles before determining the response of the medium," said Olvera de la Cruz. "The dielectric response and the motion of the charged particles are inherently coupled, and our model mirrors that."

The researchers formulated a new function that gives the correct response of the medium and produces the true energy of the charged particles. This enabled them to update the position of the charged particles and the medium's response in the same simulation time step. Within this theoretical framework and simulation design, they were able to attack problems that were previously intractable.

Story Source:

The above story is reprinted from materials provided by **Northwestern University** .

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Journal Reference:

1. Vikram Jadhao, Francisco Solis, Monica de la Cruz. **Simulation of Charged Systems in Heterogeneous Dielectric Media via a True Energy Functional** .
Physical Review Letters , 2012; 109 (22) DOI: 10.1103/PhysRevLett.109.223905

Note: If no author is given, the source is cited instead.