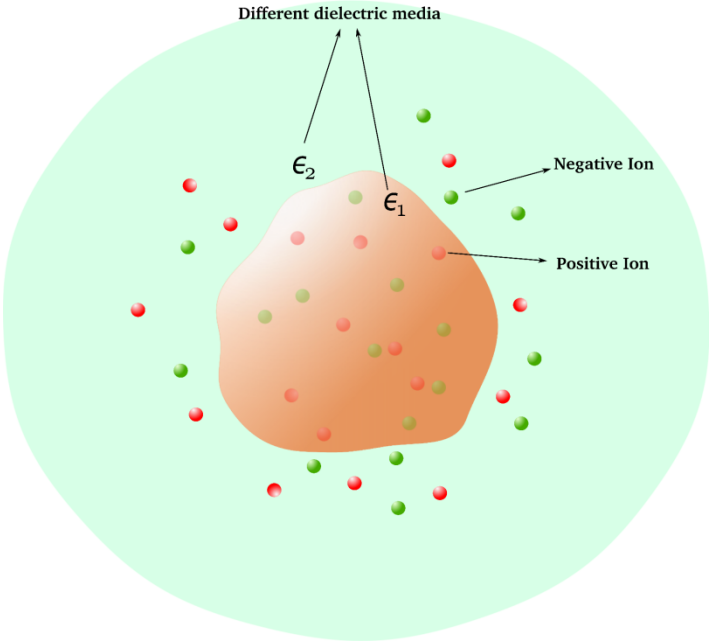
Simulation of charged systems in heterogeneous dielectric media via a true energy functional

Vikram Jadhao[1], Francisco Solis[2], Monica Olvera de la Cruz[1]

[1]Northwestern Univ., [2]Arizona State Univ.

In biology and materials, media with different dielectric properties form interfaces and harbor ions. For example, in biology we see a protein (one dielectric medium) surrounded by an aqueous solution (another medium) that contains ions; or we find ions channeling across a cell membrane separating the intracellular dielectric medium from the extracellular one. Similarly many soft materials such as charged nanoparticles exhibit an interface between two different dielectric media. In simulation of such systems, a major challenge is to accurately measure the effects of the dielectric medium on the charges and the effects of the charges on the medium's dielectric response.



Typically, such information comes at the expense of solving the Poisson equation, an equation that governs the motion of the charges, at **each** step of the simulation, leading to enormous computational costs. Our work shows that such an explicit solution of the Poisson equation can be entirely avoided in simulations that originate from a judiciously designed variational formulation; leading to tremendous speed-ups in computing. By formulating the electrostatic problem as an energy minimizing problem, with a variational principle based on an energy functional of the density of induced charges, we designed a molecular dynamics simulation method that accurately solves the Poisson equation *on-the-fly*, in tandem with the energy-conserving update of the charge configuration (Phys. Rev. Lett.; in press, 2012).

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