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A variational formulation of electrostatics for heterogeneous dielectric media[1] FRANCISCO SOLIS, Mathematical and Natural Sciences, Arizona State University, VIKRAM JADHAO, MONICA OLVERA DE LA CRUZ, Materials Science and Engineering, Northwestern University — Many biological and synthetic soft matter systems involve fixed or mobile charges. The electrostatic interactions between these charges often play crucial roles in determining the structural properties and physical behavior of these systems. Coarse-graining of the properties of these systems often leads to consideration of free charges embedded in a medium with varying dielectric permittivities. Investigation of the behavior of these systems by theoretical or computational methods requires, therefore, formulations of their electrostatic properties that suitably address the properties of the medium. In this talk we present a new and powerful variational formulation of the electrostatics of charged particles in heterogenous media. Our formulation replaces the electric and polarization vector fields for the induced polarization charge density at interfaces. In addition, this variational principle has the property of evaluating to the true free energy of the system at its minimum; a property not found in many other variational formulations. We discuss the application of this functional to a variety of electrostatic problems and show how it allows the development of new algorithms for simulation of charged systems in heterogeneous media.

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Francisco Solis
Mathematical and Natural Sciences, Arizona State University

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