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Towards simulation of charges in the presence of varying dielectric response VIKRAM JADHAO, Northwestern University, FRANCISCO SOLIS, Arizona State University, GUILLERMO GUERRERO-GARCIA, MONICA OLVERA DE LA CRUZ, Northwestern University — A variational formulation of electrostatics suitable for carrying out simulations of charges interacting in the presence of different dielectric media is developed. The variational principle employs the polarization charge density as the only variational field. A true energy functional is constructed to yield the correct electrostatic energy at its minimum and the correct force during the approach to the minimum. In the hope of applying the method to more realistic and complicated geometries, some numerical investigations of the variational procedure are also presented.

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