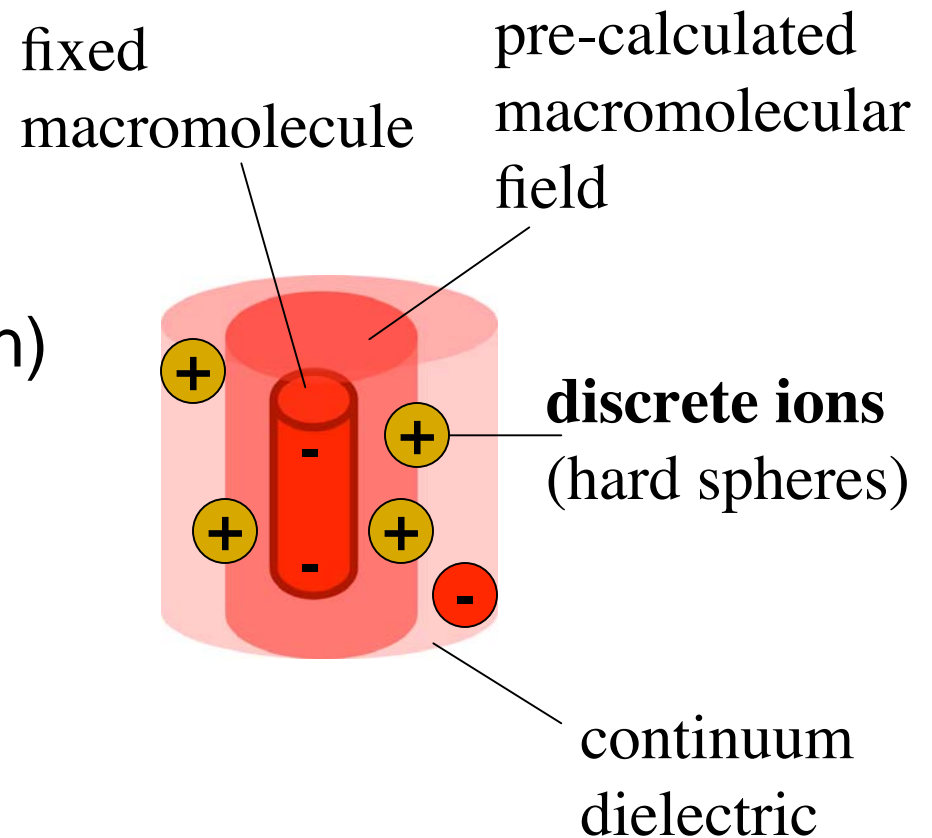


ISIM: Electrostatics simulations of the Ion Atmosphere (M. Engelhardt, C. Bruns, D. Herschlag, & V. Pande)

OVERALL GOALS:

- Develop and apply an improved predictive and quantitative model (going beyond Poisson-Boltzmann)
- Develop and apply analytical tools to examine the characteristics of the model that lead to its predictions



Normal mode Langevin dynamics (P. Petrone & V. Pande)

■ Goals

- Significantly increase speed of molecular dynamics, without using more computational power
- To be as faithful to the true kinetics as possible: predict rates, free energies, mechanism

■ Applications

- Ideally suited for conformational change
- Myosin dynamics
- RNA folding (from formed secondary structure)

