Smooth Gaussian-based dielectric function: Implementation in DelPhi

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Smooth Gaussian-based dielectric function:

Given a molecule in water phase, we applied the Gaussian equation and implemented three steps as follows to calculate the dielectric distribution of a protein from its density distribution as originally described by Nicholls and Pickup. Given a macromolecule with N atoms, the density of an atom i is represented by a Gaussian distribution (see Figure a, b):

$$\rho_i(r) = \exp[-r_i^2 / (\sigma^2 \cdot R_i^2)], \quad (1)$$

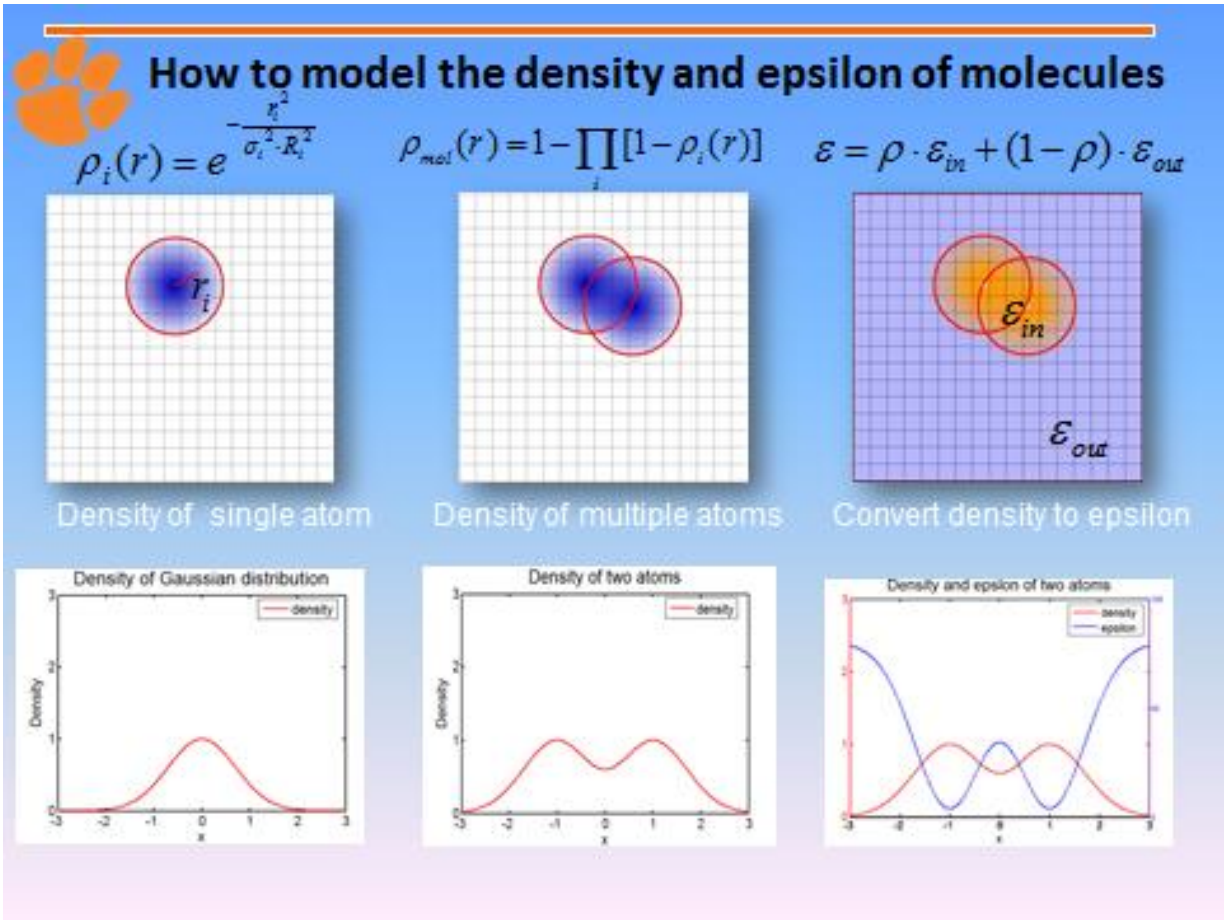
where $\rho_i(r)$ is the density at position r, r_i is the distance between the center of the atom

$$\rho_{mol}(r) = 1 - \prod_i [1 - \rho_i(r)], \quad (2)$$

where the $\rho_{mol}(r)$ denotes the density at position r coming from multiple atoms, and $\rho_i(r)$ is the density of a single atom i, which is obtained from Eq. (1). This function guarantees that the density at overlapping region is higher than the density generated by any involved single atom, but the density $\rho_{mol}(r)$ always

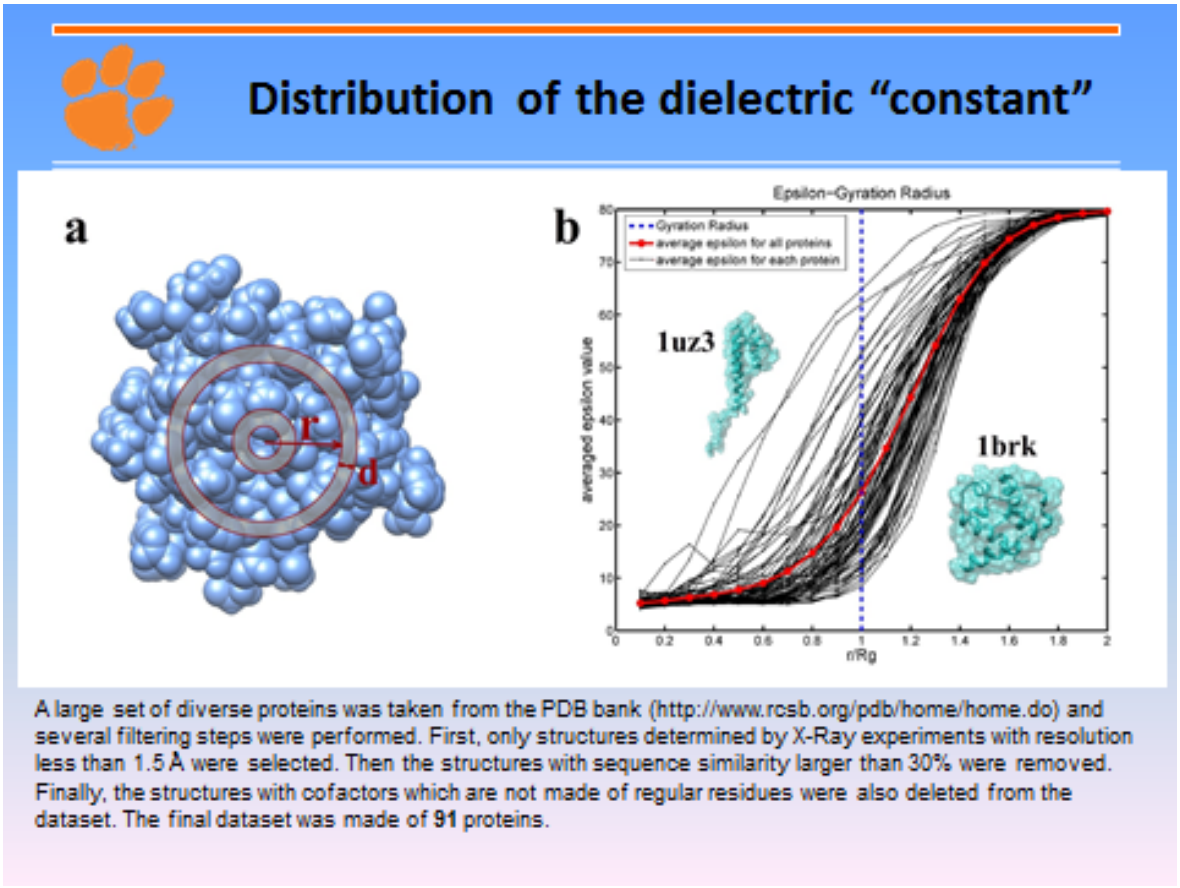
$$\varepsilon = \rho \cdot \varepsilon_{in} + (1 - \rho) \cdot \varepsilon_{out} \quad (3)$$

where ε on the left denotes the dielectric distribution function, ε_{in} denotes the reference dielectric value when the density is 1, ε_{out} denotes the reference dielectric value for water phase, and ρ is the density obtained from Eq.(2) (see Figure e,f below).



Some results:

(a) Distribution of dielectric constant with a large set of proteins



(b) Distribution of the dielectric constant in reaction center protein

Dielectric constant distribution in Gaussian presentation