FEM simulation of microwave absorption by a water drop

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The FEM electrical model of a cubic drop (edge=32 10^{-10} m) of water containing 1536 H₂0 molecules; i.e. the exact density, is solved by the association Comsol-Matlab. Each water molecule is reduced to a permanent dipole μ =1.8546 D; the O⁻ atoms are supposed to be fixed and each H⁺⁺ hydrogen is randomly oriented around its oxygen (S. Lefeuvre, O. Gomonova, chap 16, Computational Finite Element Methods in Nanotechnology, CRC Press, 2013). For each run, a Matlab script locates the 3072 points and their electrical charges, following the Comsol order, and then gives the hand to Comsol to solve three times the Poisson equation, corresponding to three boundary conditions: isolation on the six faces (said 0), isolation on 4 faces+ground and V on 2 opposite ones (said 1), isolation on 4+ ground and -V (said 2). The script collects the results, namely the coordinates of each dipole **D** and the electric field **E** corresponding to the state's 0,1,2 and makes the post-processing for instance (**E**₁-**E**₀).D to get the dipole energy. Further, it computes the mean value of the scalar products in a period of time to evaluate the mean microwave power in the drop.

It appears clearly that the H's distribution determines the solution, for instance the permittivity value; as a consequence, it has to be randomly dispersed to take into account the thermal agitation and also partly oriented by the applied field. The random distribution must be understood at the level of each H and for different runs with the same applied field **E**. A distribution is said to be "not too bad" when it produces reasonable permittivity and power.



The cloud of blue H's and green O's

Applied Electric field

One of the best result got by this method is $\varepsilon_r=97$ but all the energy conversion towards the thermic world through Boltzmann constant produces, up to now, an unbelievable result since the specific heat cannot be taken into account.