Electrostatic computations in the context of solvations models using a domain decomposition framework

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We will present recent advances in the development of discrete models of electrostatic interaction in so-called solvation models in the context of theoretical chemistry. In essence, we discretize a partial differential equation on the whole (unbounded) domain, or more precisely an interface problem between the solute and solvent domains. We decompose the solute domain into several balls and use spherical harmonics to build a discrete representation of the approximation. In this talk, after a short introduction to solvation models, I will give precise details about the discretization and show numerical results developed in the recent articles [1]–[2].

Références

[1] E. Cancs, Y. Maday, B. Stamm, *Domain decomposition for implicit solvation models*, J. Chem. Physics, Vol. 139, No. 5, pp. 054111, 2013

[2] B. Stamm, E. Cancs, F. Lipparini,Y. Maday, *A new discretization for the Polarizable Continuum Model within the domain decomposition paradigm*, J. Chem. Physics, Vol. 144, 054101, 2016

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