Fast domain decomposition methods for Continuum Solvation: theoretical foundation of the algorithm

Benjamin Stamm, Université Pierre et Marie Curie et CNRS

Filippo Lipparini, Université Pierre et Marie Curie

Eric Cancès, École des Ponts ParisTech

Yvon Maday, Université Pierre et Marie Curie

Benedetta Mennucci, Università di Pisa

In this communication, we present the theoretical foundation of the ddCOSMO algorithm, recently proposed by some of use [1, 2] to solve the equations associated with The COnductor-like Screening MOdel (COSMO), a popular solvation model. The underlying mathematical problem consists of solving Laplace's equation with non-homogeneous Dirichlet boundary conditions in a very complicated domain that is defined by the cavity of a molecule that can consist of the union of several ten-thousand of spheres. We start with giving a introduction to the chemical context and then present the algorithm that is based on a domain decomposition approach for integral equations that can be efficiently solved using spherical harmonics.

Références

[1] E. Cancès, Y. Maday, B. Stamm, *Domain decomposition for implicit solvation models*, J. Chem. Phys. 139, 54111, 2013.

[2] F. Lipparini, B. Stamm, E. Cancès, Y. Maday, B. Mennucci, *Fast domain decomposition algorithm for continuum solvation models: energy and first derivatives*, J. Chem. Theory Comput. 9, 3637-3648, 2013.

Benjamin Stamm, LJLL, UPMC Paris 06, 4, Place Jussieu, 75005 Paris, France
stamm@ann.jussieu.fr
Filippo Lipparini, ICS, LJLL et LCT, UPMC Paris 06, 4, Place Jussieu, 75005 Paris, France
filippo.lipparini@courriel.upmc.fr
Eric Cancès, CERMICS, École des Ponts et INRIA, 6 & 8 Avenue Blaise Pascal, 77455 Marne la Vallée, France
cances@cermics.enpc.fr
Yvon Maday, LJLL, UPMC Paris 06, 4, Place Jussieu, 75005 Paris, France
maday@ann.jussieu.fr
Benedetta Mennucci, Dipartimento di Chimica e Chimica Industriale, Università di Pisa, Via Risorgimento 35, 56126 Pisa, Italy
bene@dcci.unipi.it