Fast domain decomposition methods for Continuum Solvation: efficient and parallel implementation

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In this communication, we present an efficient and parallel implementation 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. Such an implementation has been coupled with both classical molecular dynamics codes (TINKER) and quantum chemistry packages (GAUSSIAN): with respect to previous, existing discretizations, ddCOSMO is at least two orders of magnitude faster, paving the way to routine applications with large molecules. Some first, preliminary applications are shown.

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.

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