Fast 3DRISM algorithms for biochemical applications

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Integral equation theory of liquids (IETL) gives a possibility to describe structural and thermodynamical parameters of liquids. One of the key equations in this theory is the Ornstein-Zernike (OZ) equation. For molecular systems OZ is a six dimensional integral equation and it is still a challenging task to solve it numerically. There is a possibility to decrease the dimensionality of the problem by averaging the angular degrees of freedom. Such kind of models are Reference Interaction Sites Model (RISM) or 3D-RISM model. To apply methods of the IETL for screening of large sets of bioactive compounds one requires fast RISM and 3D-RISM implementations.

Recently it was shown that after proper parameterization, both: RISM and 3DRISM equations can be used for accurate prediction of the Hydration Free Energies (HFE) of bioactive compounds [1,2]. The structural descriptors correction (SDC) model, which is based on a combination of the RISM with several empirical corrections, substantially increases the accuracy of calculated HFEs by RISM giving the standard deviation of the error for a test set of 120 organic molecules around 1.2 kcal/mol [1]. As well, for 3D-RISM by using only the partial molar volume as a linear empirical correction (universal correction, UC) to the calculated hydration free energy, one obtain predictions of hydration free energies in excellent agreement with experiment ($R = 0.94$, $\sigma = 0.99$ kcal/mol) [2].

Recently we proposed the multigrid algorithm for solving RISM equations and showed that the proposed method is over 30 times faster than the standard one [3]. In out last paper we report the multi-grid based algorithm for the 3D-RISM equations [4]. We performed the benchmarking of the algorithm and compare its performance with the standard Picard and DIIS one-level iterative schemes. We showed that the algorithm is 24 times faster than the Picard and 3.5 times faster than the DIIS algorithms. We also benchmarked the algorithm on a set of 99 organic compounds and showed that average computation time on a standard PC is only few minutes per molecule (10-20 atoms). On the base of the Multi-grid 3DRISM algorithm the program package for 3DRISM calculations and visualizing results was developed. We will describe the main features of the programming package and algorithms which were used in it.

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