pyRISM – Python Implementation of the Reference Interaction Site Model

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The Reference Interaction Site Model (RISM) equation is a molecular integral equation theory (IET) method for molecular liquids formulated by Chandler et al.[1] and further developed over the years to apply to polar and ionic molecular liquids. It is a rigorous statistical mechanical approach to predicting liquid structure and solvation thermodynamics[2]. There are very few widely available open-source and modern implementations of the RISM equation. pyRISM is an open-source python implementation of the RISM equation. It calculates radial distribution functions and various correlation functions for neat liquids as well as solute interactions under the assumption of infinite dilution. Using the correlation functions, solvation free energy can be computed from RISM theory. It can also calculate the solvation free energy density profile of a liquid[3]. The RISM equation is a nonlinear integral equation and is treated as a fixed-point problem. This problem is solved iteratively and quickly using the Modified Direct Inversion in the Iterative Subspace (MDIIS) method for accelerating convergence. The convolutional integrals are solved with Fast Fourier Transform (FFT). NumPy[4] and SciPy[5] are utilised to make use of their built-in functions implemented in C, and Numba[6] is used to speed up any parts of the code that cannot be vectorised by NumPy. An extension of the code enables chemically accurate predictions of solvation free energies in both aqueous and organic solvents at a wide-range of temperatures using a novel deep learning derived solvation free energy functional.

REFERENCES

[1] Andersen, H. C.; Chandler, D. Optimized Cluster Expansions for Classical Fluids. I. General Theory and Variational Formulation of the Mean Spherical Model and Hard Sphere Percus-Yevick Equations. *J. Chem. Phys.* **1972**, *57* (5), 1918–1929. https://doi.org/10.1063/1.1678512.

[2] Ratkova, E. L.; Palmer, D. S.; Fedorov, M. V. Solvation Thermodynamics of Organic Molecules by the Molecular Integral Equation Theory: Approaching Chemical Accuracy. *Chem. Rev.* **2015**, *115* (13), 6312–6356. https://doi.org/10.1021/cr5000283.

[3] Palmer, D. S.; Mišin, M.; Fedorov, M. V.; Llinas, A. Fast and General Method To Predict the Physicochemical Properties of Druglike Molecules Using the Integral Equation Theory of Molecular Liquids. *Mol. Pharmaceutics* **2015**, *12* (9), 3420–3432. https://doi.org/10.1021/acs.molpharmaceut.5b00441.

[4] Harris, C. R.; Millman, K. J.; van der Walt, S. J.; Gommers, R.; Virtanen, P.; Cournapeau, D.; Wieser, E.; Taylor, J.; Berg, S.; Smith, N. J.; Kern, R.; Picus, M.; Hoyer, S.; van Kerkwijk, M. H.; Brett, M.; Haldane, A.; del Río, J. F.; Wiebe, M.; Peterson, P.; Gérard-Marchant, P.; Sheppard, K.; Reddy, T.; Weckesser, W.; Abbasi, H.; Gohlke, C.; Oliphant, T. E. Array Programming with NumPy. *Nature* **2020**, *585* (7825), 357–362. https://doi.org/10.1038/s41586-020-2649-2.

[5] Virtanen, P.; Gommers, R.; Oliphant, T. E.; Haberland, M.; Reddy, T.; Cournapeau, D.; Burovski, E.; Peterson, P.; Weckesser, W.; Bright, J.; van der Walt, S. J.; Brett, M.; Wilson, J.; Millman, K. J.; Mayorov, N.; Nelson, A. R. J.; Jones, E.; Kern, R.; Larson, E.; Carey, C. J.; Polat, İ.; Feng, Y.; Moore, E. W.; VanderPlas, J.; Laxalde, D.; Perktold, J.; Cimrman, R.; Henriksen, I.; Quintero, E. A.; Harris, C. R.; Archibald, A. M.; Ribeiro, A. H.; Pedregosa, F.; van Mulbregt, P.; SciPy 1.0 Contributors. SciPy 1.0: Fundamental Algorithms for Scientific Computing in Python. *Nature Methods* **2020**, *17*, 261–272. https://doi.org/10.1038/s41592-019-0686-2.

[6] Lam, S. K.; Pitrou, A.; Seibert, S. Numba: A LLVM-Based Python JIT Compiler. In *Proceedings of the Second Workshop on the LLVM Compiler Infrastructure in HPC*; LLVM '15; Association for Computing Machinery: New York, NY, USA, 2015. https://doi.org/10.1145/2833157.2833162.