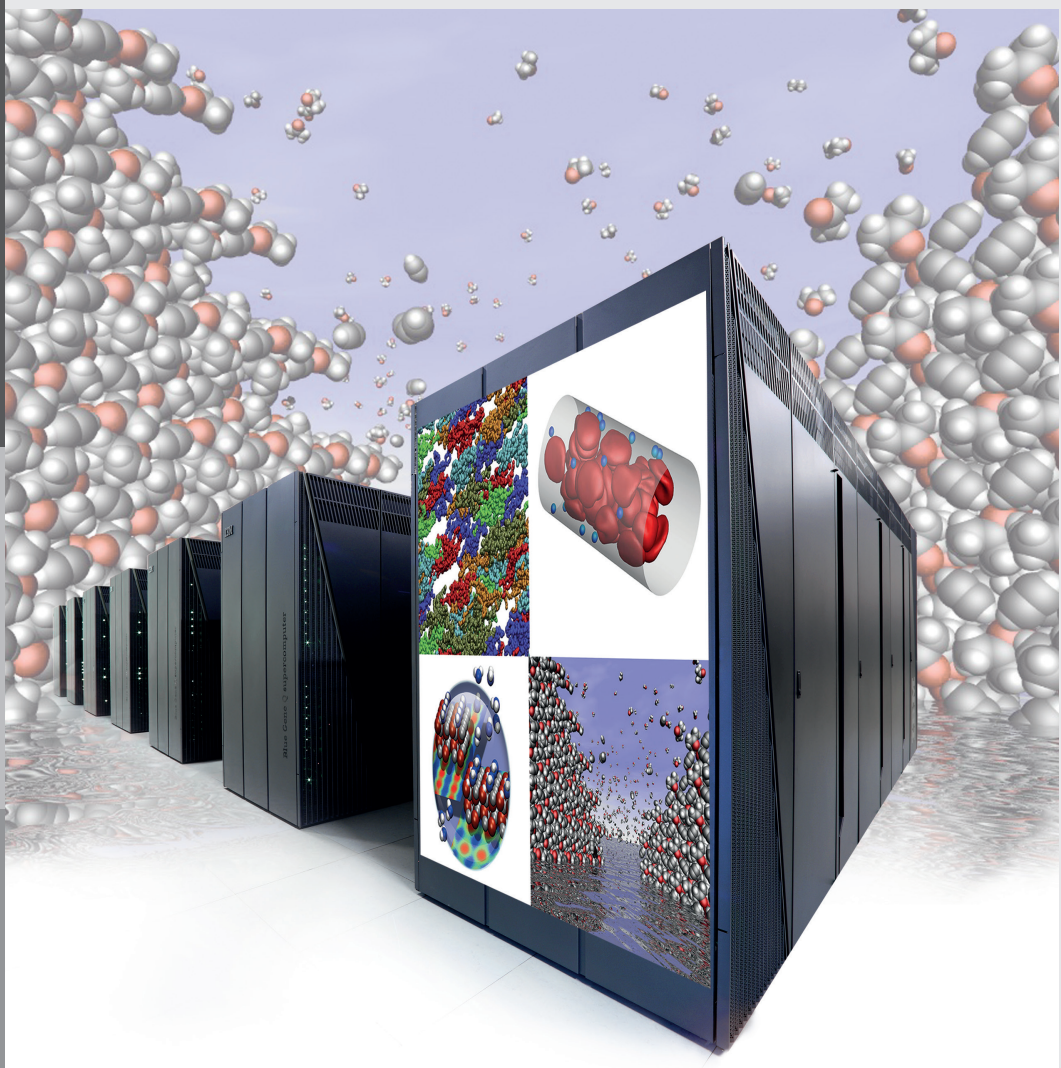

Computational Trends in Solvation and Transport in Liquids
Lecture Notes

edited by Godehard Sutmann, Johannes Grotendorst, Gerhard Gompper, Dominik Marx

Member of the Helmholtz Association

Forschungszentrum Jülich GmbH
Institute for Advanced Simulation (IAS)
Jülich Supercomputing Centre (JSC)

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Atomistic Methods

Coarse Grain and Continuum Methods

Hybrid Methods

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The majority of chemical reactions including many important industrial processes and virtually all biological activities take place within a liquid environment. Solvents, of which water is certainly the most important, are able to “solvate” molecules, thereby transferring these as “solutes” into the liquid state. Transport processes and solute-solute interactions in the solvent are then supporting structure formation, self-organization or chemical reactions. Solvents are not only able to provide a liquid phase for simple chemical reagents and the much more complex proteins; they have the additional ability to wet extended surfaces such as lipid membranes or metal electrodes, thereby creating interfaces. An in-depth understanding of solvation at a fundamental level of chemistry, physics and engineering is essential to enable major advances in key technologies for environmentally friendly technologies, e.g. to reduce pollution, to increase energy efficiency or to prevent corrosion to name but a few challenges to our modern day society. In biophysics and life sciences, water is the most important and dominant solvent, providing the basic environment for the complexity of life. Therefore, an understanding of solvation is crucial to unravel biological function in a comprehensive way.

The Lecture Notes contain the current state-of-the-art methods to treat solvation and transport on different levels of resolution. Topics include ab initio methods, atomistic and mesoscale methods for modeling accurately the solute-solvent interaction and an efficient treatment of the solvent on a mesoscopic level. Recent advances in mathematical techniques are introduced, which are fundamental for efficient treatment of solute-solvent systems. Recent trends and future directions in computational science are addressed to provide a perspective for software development and computer architectures.

This publication was edited at the Jülich Supercomputer Centre (JSC) which is an integral part of the Institute for Advanced Simulation (IAS). The IAS combines the Jülich Simulation sciences and the supercomputing facility in on organizational unit. It includes those parts of the scientific institutes at Forschungszentrum Jülich which use simulation on supercomputers as their main research methodology.

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