

Inverse Problems and Hierarchical Multiscale Modelling of Biological Matter

Alexander Lyubartsev¹ and Aatto Laaksonen^{1,2,3,4}

1-Department of Materials and Environmental Chemistry, Arrhenius Laboratory, Stockholm University, 106 91 Stockholm, Sweden

2- Centre of Advanced Research in Bionanoconjugates and Biopolymers, Petru Poni Institute of Macromolecular Chemistry, Aleea Grigore Ghica-Voda, 41A, 700487 Iasi, Romania

3- State Key Laboratory of Materials-Oriented and Chemical Engineering, Nanjing Tech University, Nanjing 210009, People's Republic of China

4- Department of Engineering Sciences and Mathematics, Division of Energy Science, Luleå University of Technology, 97187 Luleå, Sweden

aatto@mmk.su.se

In solving mathematical and physical problems we generally think that the problem can be condensed to a well-defined equation which then can be solved either analytically or numerically with the provided input data and, if necessary, applying initial and boundary conditions to limit the amount of solutions to something which makes sense and can be accepted as the correct solution. This is the typical practice in “forward” problem solving. Consequently the **solution** can be considered as the **inverse** of the problem. Indeed, it is not uncommon in Science and also in everyday life to have the “solution” without knowing what exactly did “cause” it and “how”. We take an illustrative example from Forensics with a case where a lethal crime is committed with a dead body (solution), but at the time of arrival to the crime scene the details to start to investigate are scattered all over the place. The investigators have the difficult task to mentally reverse the time to get good enough picture of the crime (problem) to start to trace the criminal and murder weapon (input) and possibly also the motive (cause). In this Chapter we discuss on how solving of the Inverse Problems is entering in Chemistry and focus on our own inverse computer modelling method to create a model (force field) from the results we already have. We explain how this method, called the Inverse Monte Carlo, can also be used for systematic hierarchical multi-scale modelling based on successive coarse-graining from first-principles to meso-scale and even further by super-coarse-graining. We show several applications of using it and also vision future prospects of hierarchical multi-scale modelling.