Chapter 15
Visualization and Minima Finding of Multidimensional Hypersurface

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ABSTRACT

Analysis of multidimensional function properties is required for industrial applications. The solution of its problems is a challenge in economics, sociology, chemistry, biology, biochemistry, and other sciences. For example, the study of the potential energy surface (PES) of a free molecule is of fundamental importance in structural chemistry because it is necessary to determine the stable conformations of a molecule and the ways of interconversion between them. However, if the PES is a function of more than three rotational coordinates, the costs of its quantum-chemical calculation rapidly increases and the problem of its graphical visualization can be hardly solved for a large number of variables. This work describes how a specially developed multidimensional interpolation procedure can contribute to solve these problems. To visualize a five dimensional (5D) hypersurface, the authors applied a special coordinate system.

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INTRODUCTION

Multidimensional data visualization as a special type of information visualization has been the subject of active research with numerous applications in a wide range of fields – from natural sciences and engineering design to industrial and financial markets in which the correlation between many attributes is of vital interest. Together with the gigantic increase of volumes of data in the world the possibility of gaining inexhaustible sources of information is growing too, enabling human knowledge to expand. However, extracting the meaningful information is a complex task when great amounts of data are presented in a plain text or in a traditional tabular form. Effective graphical presentation of data, therefore, is popular due to the fact that a person mainly gets information through visual perception. Visualization of information is the use of computer interactive visual representations of abstract and non-physical data to enhance human cognition. It aims to help users to swiftly discover and explore what is expected, as well as detect the unexpected in order to gain insight into the data. Multidimensional data are formed from a set of properties that possess a high dimension and often correlate with each other. In this sense the use of the terms multidimensional and multivariate is often ambiguous. Strictly speaking, multidimensional usually refers to a number of independent dimensions, while multivariate refers to a number of dependent variables (Bergeron et al., 1994). Hoffman considers multidimensional multivariate visualization to be a more suitable term (Hoffman et al., 2001). However, multivariate data have a high dimensionality and can be considered multidimensional because the relationships between attributes are usually not known in advance. The multidimensional will be therefore implied below in usage. Multidimensional data are analyzed by researchers, engineers, manufacturers, financial managers and various types of analysts in all aspects. Thus, multi-factor data visualization is motivated by many situations when they try to get a comprehensive understanding of data distributions and examine the relationships between different data attributes. Such a powerful visual display tool is needed to facilitate users to the identification, location, distinction, categorization, clustering, ranking, comparing or matching of base data (Wehrend et al., 1990).

For instance, in structural chemistry, one of the actual problems is determination of the energetically favorable stable conformations of a molecule (conformers) corresponding to minima (global and local) on the potential energy surface (PES) and prediction of the interconversion barriers between the conformers corresponding to local maxima, where PES is considered as a function of coordinates describing internal rotation of molecular fragments. Quantum chemical methods have become a useful tool for computations of molecular structure and, thus, for predictions of chemical properties of compounds and reaction mechanisms. It has become an alternative way to study materials before running the actual experiments that can be too difficult, too expensive or even not possible.

There are several computer software packages used in computational chemistry, such as GAUSSIAN, GAMESS, MOLPRO, SPARTAN, CFOUR, etc. The widely used program GAUSSIAN (Frisch, 2003 and the following updates) considered by most scholars to be the "industry standard" is supplemented by the visualization tool (GAUSSVIEW) which allows the graphical presentation of obtained results. In general, visualization of the PES is usually limited by two variables (3D PES). The visualization of four-dimensional and more complex hypersurfaces is still a challenge for structural chemists. Therefore, there is a need to create a reliable and affordable processor for visualization and minima finding of complex hypersurfaces. In the present work, the authors used the output of the GAUSSIAN program package.

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