EChem++ – An Object Oriented Approach to Computational Electrochemistry

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The interpretation of electrochemical data, in particular those from the application of electroanalytical techniques to molecular systems (molecular electrochemistry), is traditionally linked to computational methods. Such treatment has been termed *computational electrochemistry* [1]. It not only involves simulation [2], but also data analysis methodology (see, e.g. [3]). In a broader sense, also other computer related activities, such as computer control of electrochemical instrumentation, may be viewed as part of computational electrochemistry. Bieniasz has recently suggested a "problem solving environment" (PSE) [1] to assist experimental electrochemists in the solution of computation related tasks.

We propose to use recent software technologies such as object oriented analysis (OOA) of the overall data generation, analysis and interpretation process in electrochemical experiments as the basis for an integrated software package which may implement such an electrochemical PSE. In order to honor the underlying programming language which supports OOA and which will be used in the current work, namely C++, we chose the name EChem++ for this system. In contrast to commercial approaches, we intend to make the development of EChem++ an open source project which can be applied, extended, improved and tested freely by the electrochemical community, since the source code will be made available. The present development and implementation is under the Linux operating system, including the real-time extension RTLinux. However, no restriction to a particular operating system is intended.

Our analysis first identifies the central procedures of electrochemical research. These are as follows: The experimentalist selects a certain type of experiment, which is imposed on the electrochemical system to be investigated. Data are generated by performing the experiment, preferably under computer control. The experiment is modelled by partial differential equations with appropriate initial and boundary conditions, including (usually numerical) simulation. Experimental and simulation data are compared, resulting in estimates of interesting parameters related to the system (e.g., rate constants of chemical reactions). These results may suggest variations of the original experiment, its conditions, or the simulation which generates feedback loops.

We then define the interfaces between program modules designed to meet these tasks as well as the data streams between them, and construct various *classes* of data and related procedures to handle the tasks. By refinement of these classes in several levels, we arrive at small building blocks for the implementation of these concepts as program code. The components are then assembled to a comprehensive PSE. This approach clearly defines the underlying logical structure of the analytical process. In particular, concepts such as deriving specialized classes from more general ones is employed, and makes similarities and differences explicit. Due to the fully defined modules and data streams, it is simple to use various different implementations for a certain task. For example, various types of numerical integration techniques (finite difference, finite elements) may be employed within the same framework. In analogy, comparison between experimental and simulated data may alternatively use curve fitting, multi-parameter estimation [3], or artificial neural networks [4] within the context of the PSE. The modular and open architecture of EChem++ allows contributions of each interested electrochemist.

The presentation will discuss the basic design decisions for the software package and our first results for the application to multiple (combinatorial) cyclic voltammetry in the wells of microtiter plates.

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