Journal of Computational Interdisciplinary Sciences (2012) 3(1-2): 1-2

Printed version ISSN 1983-8409 / Online version ISSN 2177-8833
http://epacis.net
doi: 10.6062/jcis.2012.03.01.EN007

EDITORIAL NOTE

Focus issue on Computational Methods in Functional Dynamics

Marcus J.B. Hauser

This focus issue of the *Journal of Computational Interdisciplinary Sciences* is devoted to computational methods recently developed and applied in *Functional Dynamics*. Functional Dynamics is an actively pursued novel field of research, where the dynamics of a complex system constitutes an integral part of its function. Thanks to the diversity of the dynamics of complex biological, biochemical, and chemical systems, functional dynamics covers a broad scope of investigated systems and applied methods. However, they share two common principles:

First, the dynamical behaviour forms an integral part of the function of the system. This function may be biological, technical, or of any other nature. The challenge lies in unravelling both the different types of dynamic behaviour shown by the system and their underlying molecular mechanisms. An additional goal is to identify the possibly different functions associated with different types of dynamics, and how the dynamics couples with the function.

Second, the dynamics encountered in systems with functional dynamics is often complex and efforts are made to systematically construct useful models. This requires the use of nonlinear evolution equations. Often the observed dynamic behaviour is robust and does not depend essentially on the entire micro-complexity of the individual system. Hence, the task taken up in modelling often consists of reducing this complexity to a manageable level while keeping the key structures responsible for the observed behaviour.

The aim of the Focus Issue on "Computational Methods in Functional Dynamics" is to compile and present representative contributions on computational methods and procedures that have been developed over the last years and successfully applied in studies of functional dynamics. As these elaborate computational methods are very often put in a second rank in scientific papers, but lay the basis for all studies of functional dynamical systems, we wish to present them in due detail, thus bringing them into the limelight they deserve.

The present focus issue highlights areas of Fuctional Dynamics where computational methods play a significant role. In recent years substantial efforts have been made to deal with extended reaction systems, making use of graph theoretical methods to handle these large systems. These methods are presented and applied in papers that study calcium dynamics in more complex geometrical situations [1] and in complex biological settings [2], as well as in a study of the recovery of a cell from osmotic stress [3]. Methods developed for the analysis of the graph structure of reaction networks are presented in studies to assess the significance of knockout cascades in metabolic networks [4] and to generate anisotropic networks for simulations of signals spreading in excitable systems [5]. Another important line of research is concerned with the numerical simulation of the dynamical behaviour of systems showing functional dynamics. These studies often involve the development of new models and their optimization. This line of research is reflected by an article developing an elaborate model to simulate the electrodiffusion through an ion channel [6], a study of the dynamical responses of a yeast cell population to periodic perturbations [7], as well as a paper investigating the effect of a 3-dimensional geometry on the generation of patterns during electrodissolution of metals in acids [8]. Finally, we present two articles, where sophisticated computational methods were developed to analyze experimental data, thus making these data available for a vast series of numerical studies of functional dynamics of the underlying biological systems. Here, computational methods were developed to recognize and to track the cell shape of a migrating cell [9], as well as to extract the two-dimensional transportation network formed by a cellular system [10]. The latter studies make these systems readily available for further in silico studies.

The considerable progress observed in the area of *Functional Dynamics* is tightly linked to the European Science Foundation-supported Research Network Programme FUNCDYN (Functional Dynamics in Complex Chemical and Biological Systems). This programme, which was effective from 2006 to the end of 2011, promoted research on the area of Functional Dynamics and strongly encouraged the collaboration between scientists of different disciplines and laboratories. The seeds laid out by that programme are now prosperously flourishing, as demonstrated by the compilation of articles forming the present Focus Issue.

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