

Modelling cellular systems with PySCeS

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Computer modelling has become essential in the analysis and understanding of complex cellular systems. We would like to introduce a new application, developed in our group, that can be used to model such systems: PySCeS.

PySCeS has been written in the programming language Python combined with the SciPy scientific libraries. It has specifically been designed to operate on both Windows and Linux operating systems. By using a ‘toolkit’ approach we have developed PySCeS as a set of high level modules that can be used interactively in a standard Python environment, allowing for interactive use on the command line or execution of programme scripts. Along with the intrinsic functionality of a modern, object-oriented language such as Python, additional modules exist that:

- parse input files containing the model definition,
- perform a structural analysis
- follow the system’s behaviour over time,
- solve for steady state,
- calculate a control analysis,
- plot data or display it as HTML,
- access continuation routines,
- calculate elementary modes,
- read and write level 1 and 2 SBML files.

PySCeS uses a strategy of simultaneously providing access to high level, easy-to-use modelling modules as well as low-level numerical routines and has been successfully used in an advanced postgraduate teaching environment. We believe the versatile and extensible nature of PySCeS will facilitate the development of novel ways of modelling and, ultimately, understanding complex cellular functions.

PySCeS is distributed as open source software under the GNU GPL. It is available from <http://pysces.sourceforge.net>.